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B I O M O L E C U L A R C O N F O R M A T I O N

— R E T R O S P E C T S & P R O S P E C T S

(A Philosophical Review)

Dedicated to Professor John T. Edsall

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Introduction

As stated in the title, this essay is historical and philosophical — in that an attempt is made to explore the special events which led to the discipline of conformational analysis being established, and to give a bird's eye view of the development of molecular biophysics, particularly during the last three decades. Towards the end, I give suggestions as to the lines of approach for further studies that will be particularly rewarding in future, both from the point of view of their basic importance, and their relevance to the growth of biological sciences.

Necessarily, this article is based on my personal experiences during the last thirty years and therefore many investigations undertaken by me and my colleagues are picked out for illustrating the main argument. I should emphasize, however, that full references to some extremely important papers from other laboratories are not given only because this review is not intended to be exhaustive, but to picture some salient steps in the development of the subject, so that examples which are particularly familiar to me have been employed. Also, the paper is written in a conversational style, as in a delivered lecture, although I will not be talking personally in the conversation.

In his letter asking me to contribute an introductory paper for this Conversation, Dr. Ramaswamy Sarma has mentioned

how he was "a child playing in the coconut groves of Kerala" at the time when Molecular Biology was born in the late 40's and the early 50's. Although I am also a son of the same soil of Kerala, I had the good fortune of being a fully developed scientist at that time, but one who was waiting on the threshold before deciding whether to enter this new stream or not. In the late 1940's, after taking a doctorate degree working with Prof. Sir. C.V. Raman, I went to Cambridge, England and learnt at first hand the latest developments in crystallography. I had the good fortune to meet there Perutz and Kendrew who were at that time considered to have taken up an unsurmountable task, namely that of solving the structures of compounds whose molecular weights were in the region of many thousands, while solving the crystal structures of even a molecule with 20 atoms was considered an achievement. A couple of years after I returned to India, I was lucky to be made the Head of a new department in Madras, mostly devoted to research and having very little of teaching. Further, the laboratory was new and I could develop my inclinations in any direction that I wanted, subject to its being within the broad discipline of physics as it was understood then. I decided to start research on biomolecular structures as studied by methods of x-ray crystallography, the latter of which was familiar to me both from my earlier experiences with Raman and later in Cambridge.

I should perhaps explain why I was attracted to this

fascinating subject. This is not merely a personal history, but it has relevance to the reason why researchers in the field of biomolecules turned in the way they did from about the beginning of the 50's. Even in the first year of my pre-doctoral studies in the early 40's with Raman, I was attracted by two books on his shelf, namely, "Nature of the Chemical Bond" by Linus Pauling, and "Natural and Synthetic High Polymers" by Kurt Meyer. These left a profound impression on me, although at that time I was working mostly on optics and diffraction theory under Prof. Raman. I took crystal chemistry as an extra-curricular subject of study and as part of this, crystal structures came in for serious consideration. Even at that time, I used to wonder why so few of the materials that formed the building blocks of living systems were fully explored by crystallographic techniques. No doubt, the structures of silk and of cellulose and related materials were reasonably well established, by studies starting right from the 1920's, and finally confirmed by the work of Meyer and his coworkers. Similarly the pioneering studies made by Astbury on keratin, myosin etc., had clarified the fact that there exist two types of structures in the fibrous proteins, namely of the α and β types.

Alpha Helix -- the Progenitor of Molecular Biophysics

I now come to the key event that took place in the field of biomolecular structures, namely the publication of the

beautiful series of papers by Pauling and Corey (1) which appeared in the Proceedings of the National Academy of Sciences of U.S. in 1951. I read every one of them in our library (Perhaps I was the only person in Bangalore who read them all), and I was thrilled by the revelation of so much order existing in the materials of the living world. Leaving personal feelings aside, looking back from today, nobody will contradict me if I say that the enunciation of the α -helix by Pauling based on the planar peptide unit, and the crucial importance of the formation of strong and straight NH...O hydrogen bonds, which he demonstrated, were the starting point for almost all that has taken place since then in the solution of the structures of various biopolymers. Perhaps, as a crystallographer, I should mention a certain aspect about Pauling's α -helix, which those who are not crystallographers would not have appreciated so clearly. There is a "dogma" in crystallography, according to which screw symmetry can have only axes of orders 2, 3, 4 and 6. Both 5 and the higher integers, as well as non-integral values for the number (n) of units per turn, are disallowed for crystal structures. I use the word dogma, because unfortunately it has led to a delay in the realisation of the true nature of the helical symmetry in many biopolymers. It needed the clear sight and wisdom of a person of the magnitude of Pauling to realise that what is important for the stabilization of the structure of a biopolymer chain, is not crystallographic considerations, but crystal-chemical principles. In fact, although

Pauling evolved much of his ideas in chemistry, by solving the crystal structures of a large number of compounds along with his innumerable colleagues, he always had chemi . y and chemical-physical considerations in the forefront in understanding the principles regarding the nature of the three-dimensional architecture of molecules, rather than the more mundane aspects like symmetry, number of molecules per unit cell etc. Therefore, when he found that the α -helix had a non-integral number of units per turn, he had no hesitation in putting it forward as a possible structure for the polypeptide chain. I say this because, at that time when I saw Pauling's papers I was rather surprised at the fact that n was 3.6, for his α -helix, since this would not fit into a nice crystal structure with one of the classical screw axes. Even making it $18/5$ was only a way of getting over the non-integral nature.

That a non-integral number of residues per turn is not at all impossible for single helices came out even more prominently one year after the α -helix appeared, namely in 1952, when Cochran, Crick and Vand published their famous paper (2) on the Fourier transform of helical structures. I am quite sure that it was this confidence in chemical principles (as enunciated by Pauling), rather than crystallographic requirements, that removed the obstacle of a multiple of six as a necessary number of units per turn in the DNA helix (3) that Watson and Crick worked out. (I have not talked to them but it would be very interesting to know that the feeling about orthodox

crystallography was at that time on this matter. In fact, even such stalwarts like Bragg, Kendrew and Perutz missed discovering the α -helix, in their exhaustive study (4) published in 1950 (one year before Pauling's), because their emphasis was on configurations that were consistent with crystal symmetry.)

It is not very surprising that, following Pauling's alpha helix in 1951 and the DNA double helix in 1953, we were lucky in working out the triple-helical structure of collagen (5) in 1954. In fact, when Karth and I worked out the structure, we were looking for a 3-fold screw symmetry for the structure; — I shall say later about how the 3-fold symmetry was arrived at — but since we had not fully realized the non-essentialness of a crystallographic screw axis at that time, we did not look for a non-integral number of units per turn. Actually, the structure we proposed was based on a hexagonal unit cell, having 3-fold symmetry. However, all the essential physical and stereochemical requirements of the collagen structure were there in it — namely facts known from infrared dichroism, amino-acid composition, (such as fitting in of proline) and so on. However, within a year after this, when we got a good x-ray pattern of collagen right in our laboratory, we revised the value of n from -3.0 to -3.3, a non-integral number (6). This was actually done by analysing the pattern using the formulae for such a non-integral helix, as given in the paper of Cochran, Crick and Vand mentioned above. By that time, biopolymer workers had attuned themselves to non-integral numbers, although an aura

of the mystery of integers still lingers, so that, even now, many express non-integral number of units per turn as ratios of integers -- for example, 47/13 for the α -helix of poly-L-alanine, and 10/3 for collagen.

Soon after the enunciation of the collagen helix in 1954, even in the year 1955 itself, polypeptides related to collagen, like polyglycine II and polyproline, were found to have an exact three-fold axis. But, even more interesting was the fact that the unit height ($\sim 3.0 \text{ \AA}$), which Kartha and I had worked out for this helix from stereochemical considerations, was actually found to be true for these polypeptides. Since then, numerous α -helical structures and β -type structures have been demonstrated for synthetic polypeptides, and also quite a few polypeptides containing Gly and Pro, having the collagen-like helix have been observed. In view of the ubiquitous occurrence of this third type of structure, I would like to suggest the name γ -structure as a generic term for all polypeptide structures having a collagen-like configuration -- irrespective of whether the number of units per turn is exactly three or not. The term γ -helix will signify a peptide chain configuration having a left-handed helix close to three units per turn, and a unit height of the order of 3 \AA . (There is likely to be no confusion with the γ -helix that Pauling put forward in 1951, since we know from energy considerations that this is unlikely to occur and as it has also never been observed.) In terms of the (ϕ, ψ) -angles, the α -, β - and γ -structures will lie in

the vicinity of (-60°, -60°), (-120°, 120°), (-60°, 120°).
(See Table 1 below).

Generation of new ideas and their detailed application:

Since this essay is philosophical in tone, I would like to discuss certain aspects related to the enunciation of completely new ideas like the α -helix, which is the result of inspired thought. Although it is likely that an "inspiration" is necessary for the breakthrough to occur, it has also to depend, to a large extent, upon previously existing observational data and theoretical ideas. Also, it is quite likely that, although the essential principles of the new idea are absolutely correct and indisputable, the details that are worked out regarding this need not necessarily be all correct. I shall illustrate this by a re-examination of what happened in the 1950's. This period is sufficiently far off for us to make a retrospective historical survey, and I am doing this here with the purpose of pointing out that, when new theories are put forward, we should not criticise them too much, just because some consequences of the theory are obviously incorrect. In spite of this, the positive aspect must be given credit, even though there may be negative consequences. The latter could often be remedied by making suitable improvements or modifications in the theory.

This is seen very well by a reexamination of the 1951 series of papers by Pauling. Even in his first paper, he mentions about a helix which he designates as the γ -helix, at the same

time as he discusses the α -helix. However, we now know that the γ -helix has not persisted, even though the α -helix has revolutionised molecular biophysics. This does not mean that the theoretical formulation which gave rise to the γ -helix is wrong. It only means that there were still some factors which were not completely included in the approach that led to the α -helix. I will have more to say about this later, when I deal with the criteria that could discriminate between a good biomolecular structure and a bad one. In fact, the α -helix coordinates as given by Pauling in 1951, would not be acceptable today, because they do not satisfy the contact criteria that we now adopt. One finds the same thing about the early coordinate data of the DNA helix that was worked out by Wilkins. The same thing is true of the first coordinates of the correct non-integral helix of collagen (5) which Kartha and I worked out and which was criticized, on this point, by Rich and Crick. However, all these three structures are essentially correct, as is shown by the fact that, when better data and better mathematical techniques were available, they could be used to refine all these structures to ones which are perfectly good from the point of view of their packing energy. The point I wish to make here is that, in retrospect, if the structures of the α -helix, the DNA helix, and the collagen helix, as they were put forward in the 1950's, were examined from the 1980 criteria, the actual structures proposed would be declared to be unacceptable. But with the knowledge and facilities

available in 1980, they could be refined to acceptable structures, perhaps in 5 minutes of computer time.

Purely out of curiosity, I examined the literature from 1950-55 about the types of helices that had been predicted and those that have survived. I am not giving an exhaustive list, but only a few examples to show how infantile the stereochemist's approach to model-building was in those days. Thus, Pauling gave a structure for collagen in his 1951 series which was believed to fit several features of x-ray diffraction, infrared spectroscopy, and so on, and yet was nowhere near the correct structure. It even contained cis residues, which were shown not to exist by infrared studies, later in 1954. Again Crick (probably influenced by the double helical nature of DNA) proposed a double helix for collagen in 1954 and showed by an optical diffractometer study that it fits the x-ray diffraction pattern for collagen. This again contained a cis peptide unit not present in collagen and the only feature in which it agrees with the finally determined structure is that the NH...O hydrogen bonds are nearly at right angles to the helical axis, as given by the infrared dichroism studies. During that time (1950-54) several other wrong structures for collagen were given which I do not wish to quote here, but may be seen from my article in the "Treatise of collagen" Vol. I (7).

Coming to feather keratin, Pauling, influenced again by the success of his α -helix for α -keratin, proposed that feather keratin consists of α -helices. Here also, we in Madras were

influenced by the collagen-helix, and proposed that feather keratin contains a collagen-like structure for its helical-chain. We were encouraged in this, to a large extent, by measurements on the optical rotation $[\alpha]_D$ of soluble feather keratin, which give a value of -400° , as compared with -350° for collagen, -100° for the β -structure and $+100^\circ$ for the α -helix. However, both these have been shown to be wrong by later studies made by Fraser who prefers a β -structure, although it is given a super-helical left-handed twist, which will bring it close to the collagen orientation on the average.

Since we are talking of helices, I might perhaps add a few lines about the different types that have observed so far for polypeptides. We have already considered three well-known ones namely, α -helix occurring in α -keratin and myosin, the β -helix which occurs in β -keratin and silk, and the γ -helix which occurs in collagen and polypeptides related to it. The question arises whether there are any more standard helices for the L-polypeptide chain. In fact, no new types were discovered since 1954-55, until three or four years ago, when a left-handed helix, somewhat similar to the α -helix in being single-stranded and having intrachain hydrogen bonds, was proposed (8), and named as the δ -helix. This is, however, different from the left-handed α -helix, in that it has hydrogen bonds in the opposite direction to that in the α -type helices. It has interesting possibilities, and its (ϕ, ψ) -values are also given in Table 1. However, we may mention that the long delay in its

formulation was due, to a large extent, to the reluctance to question some well-accepted ideas, like the rigid planarity of the peptide unit, which hindered the search for such new possibilities. Some special experimental and theoretical stimuli were needed for it to be discovered.

Table 1

Its establishment as a possible stable structure for L-polypeptides came only after the existence of non-planarity in peptide units was established, and the energy associated with this type of distortions had been calculated from quantum chemistry. Experimental evidence that some features of it were detectable by NMR for a small sequence in the lac repressor also played an important part in its postulation (8). Very recently, Bansal and coworkers (9) have proved by energy minimization that the so-called ω -helix, with $n = -4$, supposed to occur for poly- β -benzyl-L-aspartate, is really the δ -helix with $n = -4$, since the latter is lower in energy than the former by about 10 k cal/mole per residue.

Different Approaches in Scientific Research, as shown by Examples in Biopolymer Conformation.

Since this article deals with some general aspects of scientific research with special reference to biopolymer structures, I shall now consider different ways in which such a study may be undertaken, and I shall illustrate them with expe-

Table 1. Dihedral Angle Values and Helical Parameters of the Possible all-trans polypeptide Helices

Type or Name	Dihedral Angles $\phi(^{\circ})$ $\psi(^{\circ})$ $\omega(^{\circ})$			Helical Parameters <u>n</u> $h(\text{\AA})$		Reference
<u>Alpha type - Intrachain H-bonds $j \rightarrow 1$</u>						
$2.2_7(j = 3)^a$	-78°	59°	-	2.2	2.7	(30)
$3_{10}(j = 4)^b$	-49°	-26°	small	3.1	2.0	(30)
$\alpha(j = 5)^{c,d}$	-47°	-57°	$\sim 0^{\circ}$	3.6	1.5	(30)
$\pi(j = 6)^b$	-53°	-70°	small	4.5	1.1	(30)
<u>Beta type^{c,d} - Interchain H-bonds*</u>						
Silk, Poly-Gly	-140°	135°	- +	2.0	3.45	(30)
β -keratin	-125°	120°	- +	2.0	3.35	(30)
<u>Gamma type - Interchain H-bonds*</u>						
(a) Hexagonal lattice						
Poly-Gly, -Pro, -Hyp ^e	-80°	150	- +	-3.0	3.1	(7)
(b) Triple-chain, coiled-coil structure*						
Collagen	-75°	160°	- +	-3.3	2.9	(7)
<u>Delta type - Intrachain H-bonds $1 \rightarrow j^*$</u>						
$\delta(j = 4)^f$	-100°	-80°	$\sim -10^{\circ}$	-4.2	1.25	(8)

* Dihedral angles rounded off to 5° .

+ A range of ω is possible for these.

- a This helix has not been observed, although the nucleus of it has been observed for a pair of peptide units.
- b This occurs occasionally in globular proteins.
- c Common in globular proteins.
- d Widely prevalent for polypeptide chains and in fibrous proteins.
- e Occurs also for mixed polypeptides of these, especially having the sequence $(\text{Gly-X-Y})_n$, with X or Y as Pro or Hyp.
- f Poly-L-diamino-propionic acid, poly- β -benzyl-L-aspartate, and related polypeptides, probably have this helical structure.

riences in our own laboratory. In particular, I shall summarize the collagen structure story in which luck played a great part, and the (ϕ, ψ) -plot discovery, which was completely preplanned and was the culmination of a programmed approach.

(a) Leap in the Dark

As I told you, our interest in collagen arose from an attempt to follow up some of the problems arising from the studies that Pauling and Corey had initiated; but I did not know where to start or how to go about getting a biological fibre specimen. It was a curious coincidence that both these difficulties were simultaneously resolved for us as a result of the visit of Professor Bernal to the Madras University some time in 1952, or 1953, soon after I had joined there. He told me (confidentially, of course) that he did not believe that the Pauling-Corey structure for collagen was correct and indicated that the problem was wide open. He even went one step further, and told me that, right in the Biochemistry Department of Madras University, which was only one floor above ours, they had a sample of collagen — actually it was elastoidin (shark fin ray collagen) — whose amino-acid composition had been determined by Prof. Damodaran and colleagues of that department.

As soon as Bernal left, I contacted Biochemistry and got

this material. It was my first experience of mounting a biological fibre on an x-ray camera and taking its fibre diagram. The picture showed, in principle, all that had been stated in the literature for collagen; but it was too diffuse. I did not know at that time that this material really consisted of two parts (which has been found out only during the last ten years, or so), one of which is truly collagen-like, while the other is some other protein rich in tyrosine. However, I could see that this fibre pattern was not good enough for our studies, and we therefore looked up, in great detail, the literature connected with x-ray diffraction pattern of collagen. We then learnt that the best patterns had been obtained using kangaroo tail tendon. But where to go for a kangaroo in India? A solution to this also became possible very quickly, because only a few months earlier, the Central Leather Research Institute had been established in Madras and, as luck would have it, this was also next door to our University campus. I need not tell you that the protein in leather is almost completely collagen. Therefore, I went to the Deputy Director of that Institute, Dr. Y. Nayudamma, and asked him whether he could give me a good fibre of collagen suitable for x-ray studies, and in passing, I told him "Kangaroo tail tendon will do very well". I then forgot about it; but imagine my surprise when only six weeks later, I received a tube containing just this material. Apparently, Dr. Nayudamma had contacts with leather technologists in Australia, and through

them, he had obtained this material.

The very next day we took the diffraction pattern of this in our fibre camera and we were delighted when we found that this was as good as any reported photograph of the x-ray pattern of collagen. But it was more than that, because this was our own photograph, and we could measure it in whatever way we wanted. In fact, we took photographs mounting the fibre at various angles to the x-ray beam, and careful measurements made on these provided very useful data for evolving the finer details of the structure of collagen.

Perhaps one more contributing factor to the success of my studies on collagen should be mentioned, and that is the fact that Gopinath Kartha, who had obtained his Ph.D from Bangalore working with me, had come over to Madras to continue his post-doctoral studies. He was a trained crystallographer and this greatly helped in making this investigation. On the other hand, the laboratory in Madras was new and we had practically no crystal models, or material for making such models. In building a structure, therefore, we had to use the ribs of coconut leaves which were used for linking peptide units, which were drawn on cardboard, joined with one another using soft wax at the α -atoms. The structure so obtained was very crude; but even so, the possibility of three-dimensional visualization was very useful, although this approach was supplemented by planar drawings of projections, and by calculations. Of course, we had several suggestive ideas from

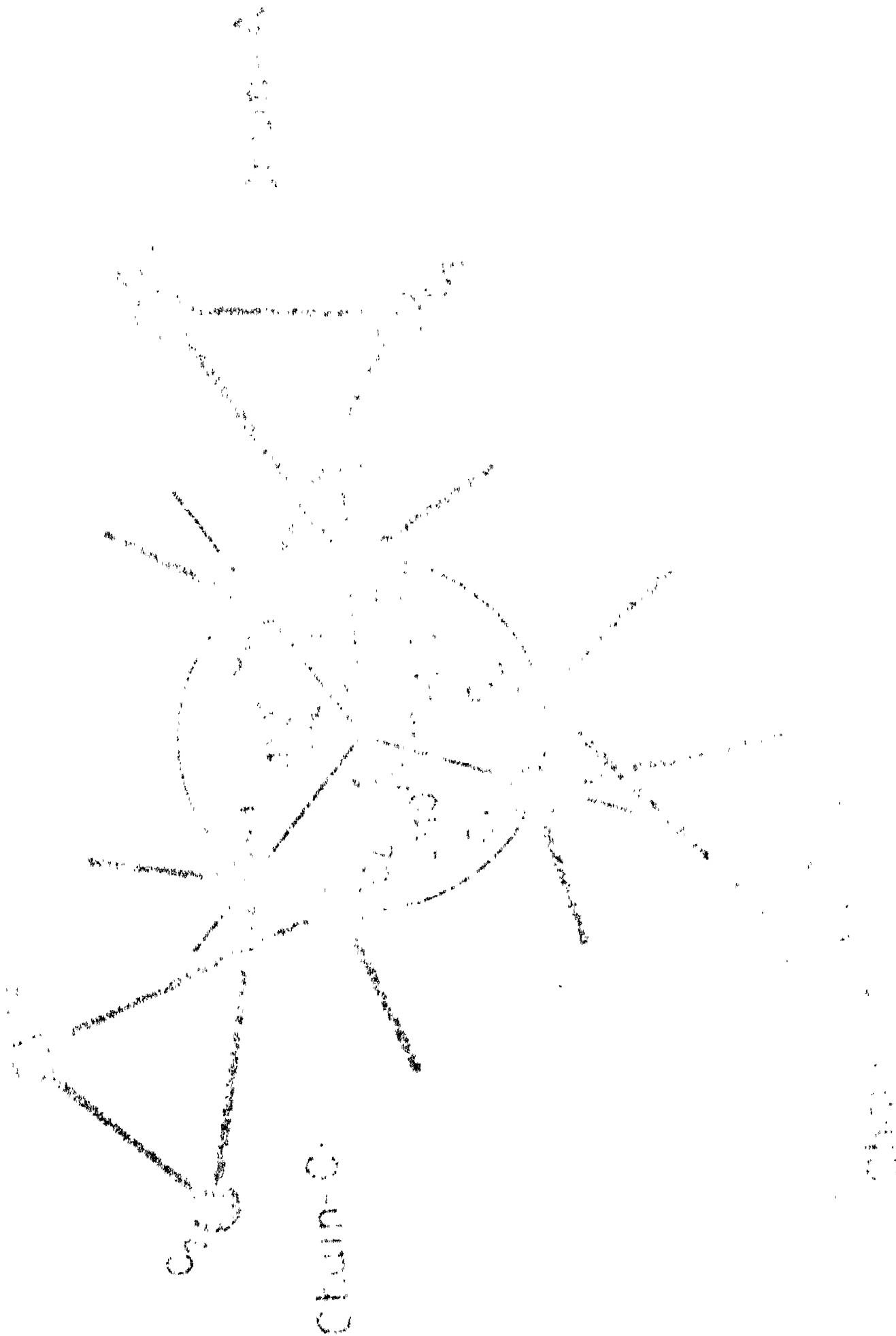
the literature. The essence of the planar peptide unit, as enunciated by Pauling, was at the core of it, and following it was the fact that only trans peptide units can occur in the structure, as indicated by infrared data published about that time (1954) by Badger and Pullin. We thus ruled out cis peptide units, which had been used by Astbury, by Pauling, and by Crick, in their earlier attempts at building the collagen structure. This was/^a very happy choice, because, as you all know now, cis peptides do occasionally occur in proteins and, even now in 1981, we do not know why --- I shall explain this later in relation to a recent study of ours.

The occurrence of glycine as one-third of the total number of residues is the most conspicuous and universal feature of collagen from all sources. We took that as the foundation for our structure, namely that glycine must occur at a positions in the helix where no other side group (not even CH_3 as in alanine) can exist. We took the clue from Pauling that glycine occurs at every third position, which very naturally explains the 1/3 frequency of this amino acid. (There was no clear-cut evidence either for, or against, this assumption at that time.) As infrared data indicated, the NH and CO bonds are nearly at right angles to the fibre axis. With these in our mind and also employing a crude interpretation of the x-ray pattern, that it had a left-handed 3-fold screw with approximately 3 \AA as the repeating unit, we worked out the first structure. The left-handedness arises because the rigid ring of proline cannot fit

it otherwise. Thus, the structure could readily incorporate proline and hydroxyproline (specific to collagen), without any modification of the stereochemistry demanded by the other considerations.

This was published in Nature in 1954 by Kartha and me (5). By this time a young student, Ambadi, who is an excellent experimenter had taken inclined-beam x-ray photographs of collagen and when we analyzed this according to the formula of Cochran, Crick and Vand it led us unmistakably to the non-integral number 3.3, or something very close to it, as the number of units per turn. We therefore re-examined the 1954 structure. The presence of proline, with the rigid side-chain-backbone interaction, demanded that the modified structure can have only one pattern — namely a left-handed minor helix, with a right-handed super-helical twist of about 30° ($\sim 0.3/3.3 = 1/11$ of a full turn of 360° .) The details of this and the method of understanding the collagen structure is given in my two articles (a) in Treatise on Collagen, Vol.I (7), and (b) Biochemistry of Collagen, 1976 (10). So I shall not say more about this, since we are not discussing collagen as such, but with the approaches that helped us in this study. However, the architectural scheme of the backbone in collagen is shown in Fig. 1.

Fig.1. Essential Backbone Architecture of the Collagen Triple Helix, projected on to a plane normal to the Helical Axis.



(b) Ignorance is Bliss

If I may say so, a certain naivette on our part helped us in getting the solution, because we did not know enough about the literature in the protein field to be influenced by any other considerations. For instance, by that time Gustavson had shown that hydroxyproline is very important for collagen and that it leads to greater thermal stability to the collagen fibre. Also, an early study by Stetten (11) had indicated that only proline is incorporated in collagen and hydroxyproline is not incorporated, so that hydroxylation should take place after incorporation of proline. If we had known all these, we would have run after the presence of hydroxyproline as one of the essential features of the collagen molecular structure, (which it certainly is from the chemical point of view, and even from the physical point of view, as we ourselves proved in the early 1970's.) However, the work we did in 1972-73 could never have been done in the 50's for absence of other vital information, and it would have been a wild goose chase. Thus, as the saying goes, "Ignorance is bliss" ! As a matter of fact, none of the other workers investigating collagen at that time also gave a moment's thought to hydroxyproline, although they all, like us, found the right modification of the triple helix which will incorporate proline and which will fit the x-ray pattern, namely to make $n \approx -3.3$, or $-10/3$, for the individual minor helices.

(c) Pre-planned Attack

I shall compare the way in which the collagen work was

done, namely by taking a leap into the dark, with a thoroughly planned investigation of ours, leading to the enunciation of the (ϕ , ψ)-plot, which came as a result of years of concerted effort. It is a long story. Sometime after '55, collagen had become a finished product. Kartha left for Europe and U.S.A. and it was not very profitable to refine the structure, since the x-ray pattern did not have too much of information for this purpose. We therefore turned into biomolecular crystallography and studied the crystal structures of a number of amino acids. While doing this, we developed some new techniques in crystallography which is not relevant to the present article.

However, in working out the structures of these amino acids, we had to study the available literature on amino acid and peptide crystal structures. Also Sasisekharan, who had joined me for his doctoral work, did a thorough refinement of the collagen structure, purely from theory, namely the point of view of getting a "good" structure free of "bad contacts". The attempt was empirical, and we used the information we could gather about various amino-acid conformations from the available literature. Again, I should mention that no models were used in this; it was all drawings and calculations. In fact, every structure we studied was looked at, only as a projection drawn on paper. In this way, we got thoroughly experienced in changing angles between bonds by one degree, or less, and changing the distances between atoms by one-tenth of an Å. However, in building such structures, we always met a stumbling block and

that was that we did not know how to assess whether a structure was good or not good — that is to say we had no quantitative criteria for checking whether a theoretically proposed structure of a biomolecule, or biopolymer, was acceptable or not.

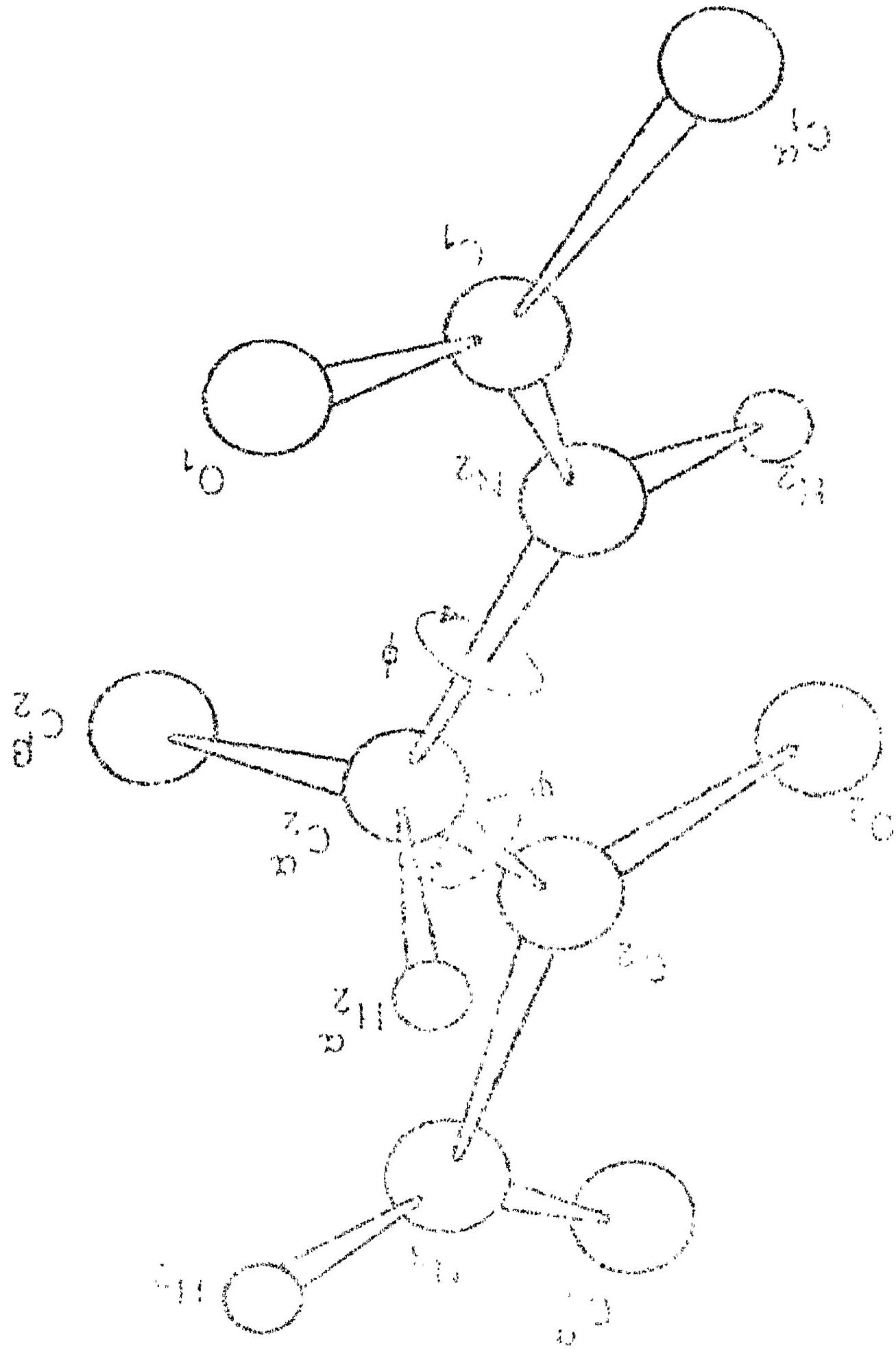
This led us to an analysis of available crystal structures on peptides and amino acids. Not surprisingly, most of these were from Pauling's own laboratory at Caltech; but the data had not been analysed in the way that we did — namely to find out what were the ranges of the variation of different parameters, such as bond length, bond angles, and so on. The values of covalent bond lengths and bond angles were pretty well known. But what are the limiting distances for Van der Waals contacts were completely unknown at that time. In fact, the literature on crystal structures never listed all the nonbonded contacts except what the author "felt" was a short contact, and we had to calculate these for various structures that were available.

We did this, although we had only desk calculators for this purpose. About that time, another young man, Ramakrishnan, had also joined for his doctorate, and Sasisekharan had practically completed his doctoral work, so that I had a young person to whom the crude labour could be given, and another who could help in the refined analysis of the data. Very soon, in the early 1960's we came at certain regularities in the limiting contacts, which we readily verified were satisfactory and

agreed with almost all structures known at that time. But the main question still remained, as to how exactly systematic variations could be made in building up the structure of a molecule, for the purpose of testing for freedom from bad contacts. We knew, no doubt, that bond angles could not be changed very much, and luckily, we did not press in this direction, because it would have been a fruitless task.

However, during Sasisekharan's approach to the refinement of the collagen structure, we had adopted a technique which involved rotations about certain lines. In this case, it was the "virtual bond" $C_1^\alpha — C_2^\alpha$ in a peptide unit with a rigid planar structure. What we did was to rotate the peptide unit about this line over a range of angles that permitted the interbond angles at the C^α -atom to remain within the allowed range of $110^\circ \pm 3^\circ$. While this was a reasonable solution, it was extremely cumbersome and we wanted to improve on this. It was as a result of this long search for a satisfactory and convenient way of building a peptide structure, that we were led finally to the very simple idea that these rotations could be taken to occur about the covalent bonds themselves which join each C^α -atom with the next atom in the chain, namely the two bonds $C^\alpha — C'$ and $N — C^\alpha$, as shown in Fig. 2.

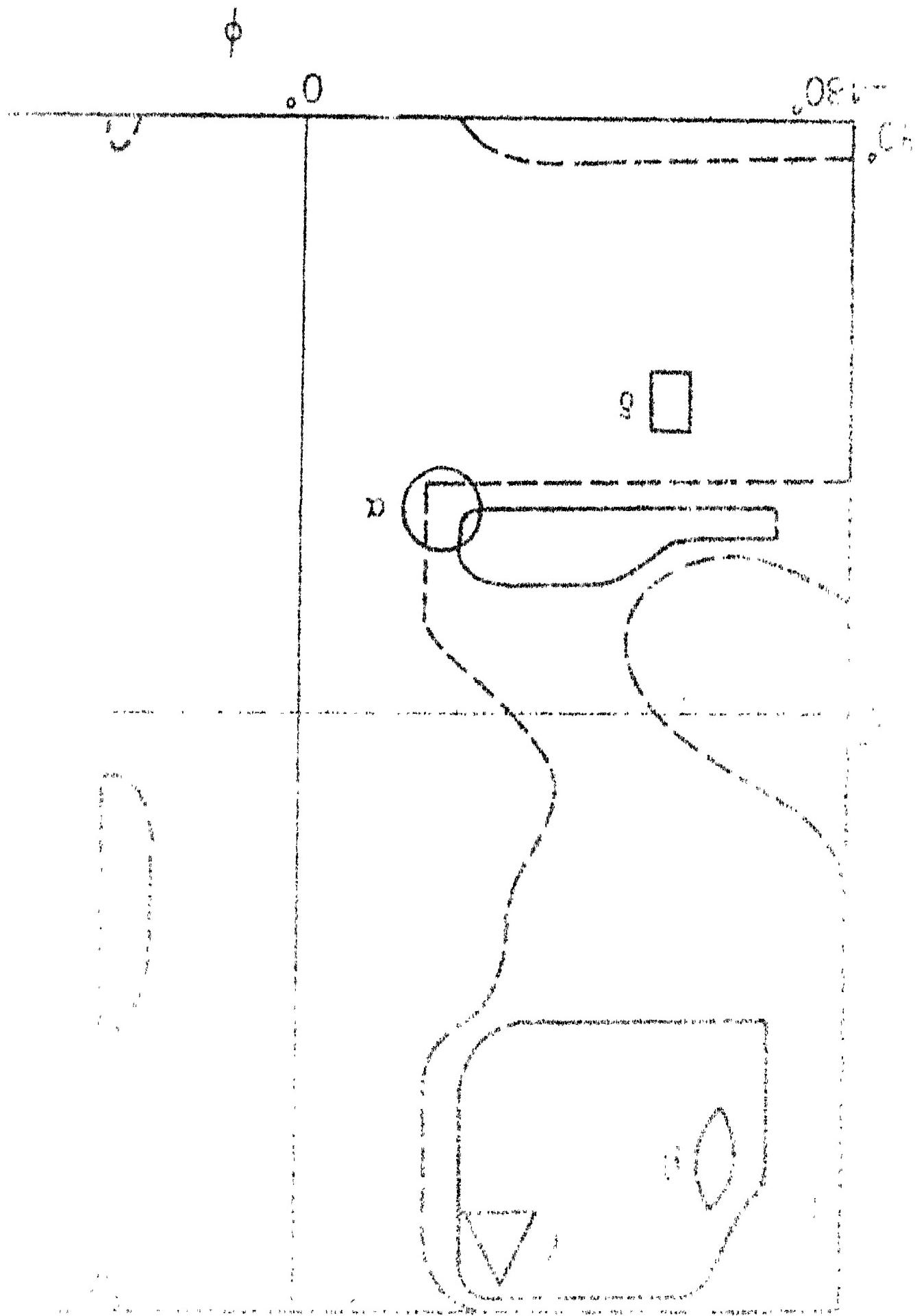
Fig.2. Diagram showing the Dihedral Angles ϕ and ψ (See later for the nature of ω).



The evolution of this idea took a couple of years. In the beginning, we found out only the effects of the restriction of the backbone atom-atom nonbonded distances and this was published in the volume reporting the symposium on Collagen (12) held at the Leather Research Institute in 1961. Very soon, this was extended to the effect of side-chain-backbone contacts also — with only the CH_3 group of alanine being included for the side chain. The work was back-breaking, and it took almost 6 months for Ramakrishnan to obtain the complete data, once the procedure was quite clear. But, when the data were plotted in what we now call as the (ϕ, ψ) -map, the results were really rewarding. We could see at once that every structure that had been determined at that time had its ϕ - and ψ -values within the ranges that we had marked in this map using the contact criteria. This was published in 1963 in the Journal of Molecular Biology (13).

Fig.3. The (ϕ, ψ) -plot, according to the IUPAC-IUB conventions.

I have often been asked as to how confident we were about the contact criteria. As shown in Fig.3, two sets of contacts were given — namely the "normal limits", and what we now call "extreme limits". This was necessary, because when we examined the observed crystal structures, we found that most of the non-bonded contacts were above the normal limits, but in some rare examples, these were violated appreciably. The choice as to where the limit of the normal contacts came, and where the limit



of the extreme contacts should be put, was empirical, based purely on our judgement. But, it is really gratifying to note that, even now, more than 25 years after the formulation was made, the contact distances which we had indicated have remained practically unchanged, and the map drawn in '62-'63 is still valid. The one and only improvement, perhaps, is the recognition, in recent years, that the C...H and H...H contacts could be softened a little more, by reducing their limiting values by 0.1 \AA . I shall say something more about this softening, at a later stage.

What I wish to emphasize is that, very often, a result of importance like the present one occurs only as a result of a long and pains-taking search. In our case, we did not know what the result of the search would be; but we wanted some rule that we could use, whereby we could say when a structure is good and acceptable and when it is not. In fact, I was very pleased when Prof. Pauling, in his discussions with us when he came to Madras in 1967, said that, in Caltech, they had studied more amino acid and peptide structures before 1960 than in any other laboratory, and rightfully the (ϕ, ψ) -map should have been discovered in Caltech.

(d) Strategy of waiting for the right time to come.

Now, I shall illustrate a type of research in which one has to wait a long period for the right type of information to become available, so as to complete the line of approach that was adopted.

It was particularly so in connection with the consummation in the 1970's of the structure of collagen, postulated from theory as early as 54-55.

One of the difficult questions in the intervening period up to about 1965 was this. It appeared that the best structure that is possible for the backbone (as worked out from conformational theory) is one in which there is only one strong hydrogen bond of the type NH...OC, while experimental data indicated that there are two of them, for every three residues. In fact, in the early structure which we proposed there were two. But, calculations of energy indicated that, although it had an extra hydrogen bond, the short contacts introduced thereby destabilise the structure, and the two-bonded structure was probably not superior to the single-hydrogen-bonded structure. In fact, there was no way of reconciling the sharp difference between the theoretical deduction of a structure with a single hydrogen bond as being the best, and the experimental observations that two hydrogen-bonded backbone NH groups could be detected for every three residues. (The third NH bond points in a direction away from the centre of the triple helix and can never form an internal backbone-backbone hydrogen bond.) I remember many occasions during conferences, at which my views were asked about this, and I used to say that one should somehow find a via media structure between those demanded by theory and by experiment.

Actually, the answer came, in just that way in 1968, from a study which I made with Chandrasekaran in Chicago, on the binding

of water to the backbone of the collagen structure (14).

Incidentally, the fact, that such a hydrogen bond between the second NH and a carbonyl oxygen via water might exist, had been stated by us in a paper published as early as 1956, but we had completely forgotten about it after that. When the subject was re-examined in 1968, Chandrasekaran had absolutely no difficulty in fitting the water molecule at a location satisfying the requirements mentioned above. In fact, I was really wonderstruck at finding that the best single-hydrogen-bonded structure that Sasisekharan had worked out, about 6 or 7 years earlier, was just right and could accomodate this extra water molecule with practically no change in the positions of any of the atoms already included. All that we had to do in Chicago was to fit in the water oxygen O_W , such that the hydrogen bonds $NH \dots O_W$ and $O_W H_W \dots OC$ were both good and strong. Incidentally, we found that one more water molecule per tripeptide could be fitted between the carbonyls, but the H-bonds were not too strong. These data were in agreement with various types of information that had been gathered about the binding of water and the format of hydrogen bonds in the collagen structure by experimental techniques. Some of them, like the one on the presence of two $NH \dots O$ bonds, were available a few years earlier, but not published, and some obtained about the same time, or a little later. However, it was the existence of the discrepancy between facts and theory that triggered our study in 1977-78.

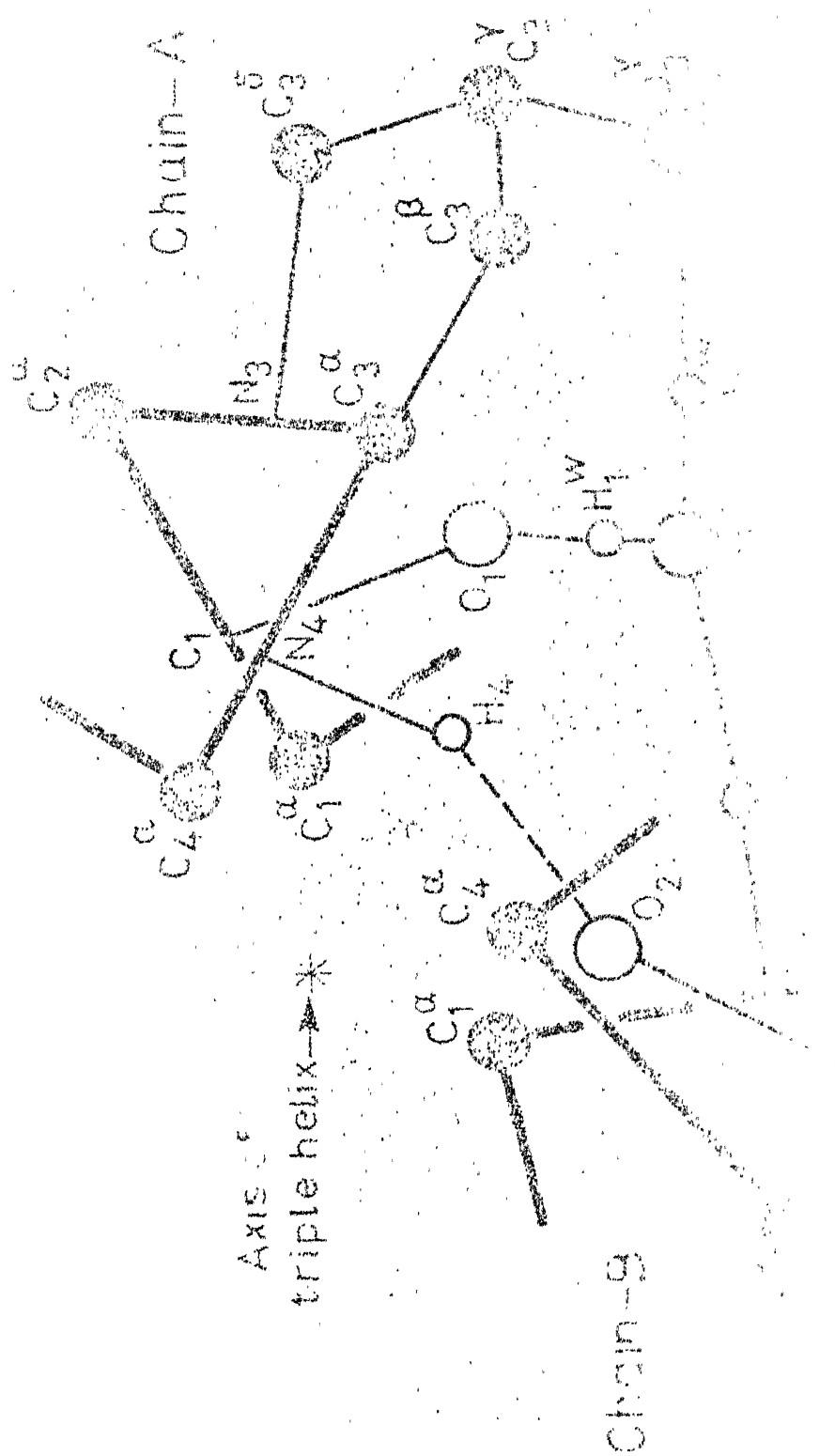
But this was not the last word. Actually, when

Chandrasekaran fitted the water molecules, I asked him the question "Would the oxygen of the same water receive a hydrogen bond from hydroxyproline if it were there?". I should mention that by that time, the importance of hydroxyproline for collagen fibril formation had been fairly well established. Unfortunately Chandrasekaran made a mistake in locating the OH group in the 4-position of the proline ring. There are two hydroxyprolines, having the OH group in the 4-cis and 4-trans configurations, the latter of which is the correct amino acid that occurs in collagen. By a strange mistake, he put it the wrong way in copying the data, from the published crystallographic structure of hydroxyproline on to collagen model, and he told me that the oxygen is pointed completely in a wrong direction and can come nowhere near the water O_W. I felt this was very unfortunate, because I was pretty sure that we had killed two birds at one shot, namely the explanation of the occurrence of two hydrogen bonds for the backbone NH's without any short contacts, and the formation, at the same time, of an extra stable hydrogen bond via hydroxyproline.

As with the earlier hydrogen bond via water proposed in 55-56, once again I completely forgot about hydroxyproline, and we did not work on collagen until 1973 when I returned from another visit for a year to Chicago and took up my assignment in the newly formed Molecular Biophysics Unit at Bangalore. It was again a lucky coincidence that a collagen biochemist, who

had worked on the hydroxylation of proline (Dr. Bhatnagar of San Francisco), should visit Bangalore just at that time, on his sabbatical leave. I told him that hydroxyproline was mysterious, and that it was not doing what it was expected to do, and I had no answer to his query. But his question stimulated me to think further about this aspect. Luckily, we had some young students who were interested in making energy calculations for biomolecule and I gave this problem to one of them. (At that time, I had no memory that I had already given it to Chandrasekaran and that he had drawn a blank). Imagine my surprise, therefore, when within one or two weeks, this student (now Dr. Manju Bansal) came back and said that the hydroxyproline makes an excellent hydrogen bond with the water O_W, placed in exactly the same location which Chandrasekaran had given for it without taking hydroxyproline into account. Immediately, we wrote a paper for Biophysica Biochemica Acta (15) saying that the role of hydroxyproline in collagen is to add extra stability to the collagen triple helix, by forming an extra hydrogen bond to the network of hydrogen bonds that is normally present. Later, the structure was energy-minimized by Bansal, and shown to be perfectly satisfactory. The structure is shown in Fig.4, in a skeletal form including only the essential atoms involved in the hydrogen-bonding network connected with hydroxyproline.

Fig.4. Hydrogen bonds between backbone atoms and the OH group of hydroxyproline via a water molecule.



Unlike the case of the firmly bound water molecules, where experimental evidence practically preceded theory, in this case experiment was simultaneous with theory. In the same year 1973 when our theoretical paper on the role of hydroxyproline was published, experimental data were also published from two laboratories showing that procollagen, which did not have the proline hydroxylated, and normal collagen, which had the proline, at position 3 in the sequence Gly-X₂-X₃, hydroxylated to form hydroxyproline, had a difference of 15°C in their melting temperatures. In fact, it turns out that if hydroxyproline were absent, collagen of bone and skin would not be stable at room temperature, and talking facetiously, I may say that you and I would not be present here for this lecture.

(e) Need for stimulus

In so far as collagen secondary structure is concerned, this is the maximum information that could be obtained, except that we may hope that, one day, someone will solve the crystal structure of a protein containing the γ -helix and get more accurate coordinates of the atoms in it. However, some five years later I had one more go at the hydroxyproline mystery. About 1975-76, I edited a book on "Biochemistry of Collagen" (10) in which I wrote a short article on the molecular structure of collagen. It also contained a very long article by Prockop on the hydroxylation of collagen, and this brought out the most interesting fact that a special enzyme called proline hydroxylase is necessary for this purpose and that this enzyme had as cofactor

ascorbic acid i.e., vitamin C. I must also add that, at about the same time, I had come to know that a component of the immune response system known as "complement C1q" had, as part of its amino acid residues sequence, a part which is highly collagen-like, in that there is glycine at every third position, a reasonable amount of proline, and also definitely presence of hydroxyproline residues in the third location X_3 mentioned earlier. From my knowledge of the collagen structure, I was absolutely sure that these were sufficient to demand that the particular portion of complement would have the collagen triple-helical structure. Even without knowing whether there were three chains or not, I would have voted for the presence of the triple helix, produced even by the same chain folding itself back and forth. Therefore, I was thrilled when I learnt in 1977 that Porter, in Oxford, had actually found that complement had a triple-helical structure and there are in fact six such rods in this huge biomolecule.

Once again, it was interesting to know that my conjecture was proved correct; but the matter stopped there, until another exciting consequence took place a few months later. This happened in Washington DC, where I was a Fogarty International Scholar at the National Institutes of Health, Bethesda. Here all the scholars were housed in a beautiful house known as "Stone House" and we met one another several times every day and there was plenty of exchange of ideas. In this way, I had a long talk with Prof. Sir George Pickering, Dean of Medicine at the University of Oxford, about various things, in the middle of which I made a comment saying that

next few months in honour of Linus Pauling's 70th birthday.

Fig.5 is the illustration that was included in this paper.

Fig.5. Flow Chart of ideas leading to the confirmation of Pauling's theory regarding vitamin C.

(f) Effect of atmosphere

I believe this is probably one of my best contributions in the field of conformational analysis, and this example clearly indicates that one must always be on the lookout for surprises, when it comes to the question of discovery. Discoveries, naturally, cannot be made to order, but just as statistics is applied in economics and in social relations, and it is said that if there is more wealth there is more happiness (although in individual cases it may not be so), in the same way, when there is a predominance of science and scientific discussion, there is certainly every chance that bright new ideas will come out. I do not remember exactly where this quotation comes from, but I am reminded of it this way — "When Greek meets Greek, there comes the spark". So, as an application of scientific philosophy towards scientific organisation, I would say there is nothing more profitable than the type of conference you are organizing, in which workers from different fields are meeting together to discuss a common subject, which is of importance to various branches of molecular biochemistry and biophysics.

VITAMIN C

is an essential
co-factor in
hydroxylation
of COLLAGEN

right's last line lesson -
stability of
COLLAGEN
imp. a helical structure
in MAGN/INDIAN

IMMUNOGLOBULIN

requires for its
action the protein
COMPLEMENT

COMPLEMENT
has in it two rows of
triple-helical proteins
containing hydroxyproline
residues

PURPLE

Both COLLAGEN and COMPLEMENT
have a triple-helical structure
and hydroxyproline residues

hence Vitamin C improves
immune Response

PAULING IS VINDICATED

Conformational Analysis

Now I turn to the general subject of conformational analysis in which, unlike in the case of collagen research, our studies were all directed towards a goal and specific problems were worked out which had been formulated earlier. This type of approach is as important for scientific research

unknown forest and searching for something beautiful whose nature even you are not aware of.

(a) Role of Conformation in Biological Activity

In this connection I am reminded of a simple illustration of what conformation is, that I give to my students. Suppose you took the human body to be a biological molecule. When this human being performs different functions, he keeps his body and arms at different angles and states of agitation. For instance, if he were swimming, his hands and legs would be rapidly going backwards and forwards. In the same way, if he is swimming in the backstroke style, his legs would make very little motion, while the hands would make a circular motion about the shoulder. If he were diving into a swimming pool, he will stretch out his hands and keep a rigid needle-like shape for his body, so that he can pierce the surface of the water with minimum resistance. On the other hand, if he is going to sleep inside a quilt, in a house without heating in winter, he will curl himself up such that his body, head, limbs etc., assume as nearly a spherical

shape as possible. (Incidentally, this is something we all do; but from physics also, this is the natural thing to do, because we reduce the surface area to a minimum and thus make heat losses as small as possible.)

What I wish to bring out by this analogy is that the shape of a molecule has very much to do with its function — in the biological systems we are interested in, and in chemical reactions in general. According to the particular type of function that it has to perform, a molecule that can assume the appropriate shape, or configuration, is selected by the living system to take that particular role.

(b) Alpha-glucose and beta-glucose polymers

Thus, for instance, cellulose is the main building block of the bulk of the plant kingdom. It forms almost 99% of its make-up and is strong and fibrous. This is achieved because the glucose residues in cellulose take a parallel orientation and an almost straight tape-like structure. The neighbouring tapes are hydrogen bonded and so are neighbouring sheets of tapes, so that we have essentially a very strong fibrous material. On the other hand, the same glucose residues, but in the α -form, cannot take up this configuration. This was one of the things that was worked out in our laboratory soon after the (ϕ, ψ) -map for proteins was discovered. In 1967, V.S.R. Rao and collaborators worked out the corresponding (ϕ, ψ) -maps for cellulose and for amylose, namely for two units of β -glucose, and for

two units of α -glucose (16). From the point of view of chemistry, these two differ minimally; but from the point of view of conformation, it is the difference between food and wood. The α -glucose chain forms a helical structure with plenty of space in between, so that the different helices cannot be easily joined to one another and each is in equilibrium in water, as in starch. On the other hand, cellulose is so well packed that it is insoluble in water.

(c) Early attempts on other biopolymers

Now we come back to the (ϕ, ψ) -map for proteins and polypeptides. As already mentioned, when tested against the known conformations at the joining C^α -atoms for the compounds that has been studied at that time, including those of the well-known α helix, β -structure, and collagen helix, they were all found to be inside the allowed ranges of the map. This gave us enormous confidence in the criteria adopted for drawing this map — namely the limiting contact distances that were used. Therefore, we went ahead and studied as many compounds as possible that we could lay our hands upon — but restricted ourselves to those that are of relevance in biological systems. As you all know, the three types of polymers that occur in biosystems are proteins, nucleic acids, and polysaccharides. We have already discussed L-polypeptides that occur in proteins. In 1967, the first typical conformational data for dihedral angles related to different linkages in nucleic acid chains were

worked out by Sasisekharan, along with his colleagues in our laboratory (17), and he extended this to various types of nucleic acid conformations that were known. In fact, as I shall briefly mention later, his great confidence in the power of these methods led him to postulate entirely new types of conformations for nucleic acid chains which were unknown previously, and which have been actually detected and found to be important, after their theoretical postulation.

In the case of polysaccharides, as mentioned above, the glucose polymers are simple to study. The extension of these to various other types of sugar polymers was systematically undertaken by Rao in our laboratory. Here also, after he had mastered the problems and peculiarities associated with the system, Rao diverted his attention towards still more complicated systems — namely proteoglycans and glycoproteins — in the late 1970's. These are compounds in which both peptide chains and sugar chains occur together. I can say, without any exaggeration, that these compounds have been studied theoretically best, perhaps, in our laboratory in Bangalore.

(d) L imitates D in penicillin

These studies on such complex materials are not merely of theoretical interest. It so turns out that the bacterial cell wall consists of peptidoglycan and one of the most important of antibiotics, namely penicillin, acts by preventing the synthesis of a portion of the peptide chains by which

different glycan chains are interlinked. It is known that the penicillin molecule is a derivative of a dipeptide L-Cys-D-Val in which, in addition a special covalent linkage occurs, leading to the formation of the β -lactam ring. Penicillin effectively prevents the combination of a peptide chain ending in D-Ala-D-Ala with the next amino acid (L-Lys, in most cases). The way it does this was originally thought to be by imitating an earlier segment of the peptide chain containing the same sequence of an L-residue followed by a D-residue, similar to what penicillin has. However, Rao (18) was able to show that the L-D sequence in penicillin really imitates the D-Ala-D-Ala sequence in the peptide chain, which is made possible because of the special β -lactam linkage that penicillin has. The similarity of the penicillin molecule and a stable conformation of the D-Ala-D-Ala fragment which it simulates, is shown in Fig.6, which has been specially prepared by Rao for this lecture. In as many as five places, the corresponding atoms in the two cases occupy the same relative three-dimensional configuration. In fact, this is perhaps the best-illustrated example of a "competitive inhibitor" of an enzyme, and I consider this as one of the most outstanding achievements of conformational theory.

Fig.6. "L imitates D" in penicillin. The black dots represent atoms in the penicillin molecule, while the open circles stand for those in the substrate. Now the close similarity in conformation between the two shown by the locations of corresponding atoms at the five places marked a, b, c, d, e.

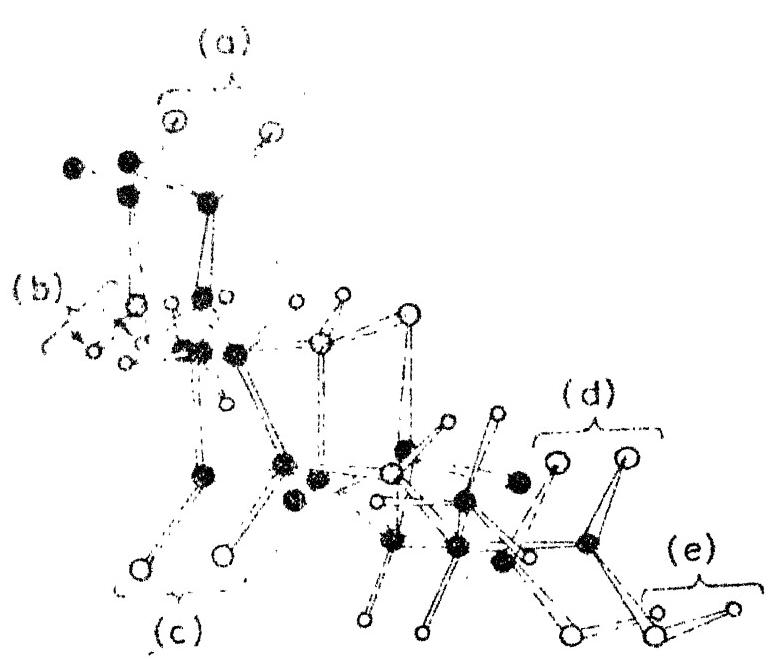
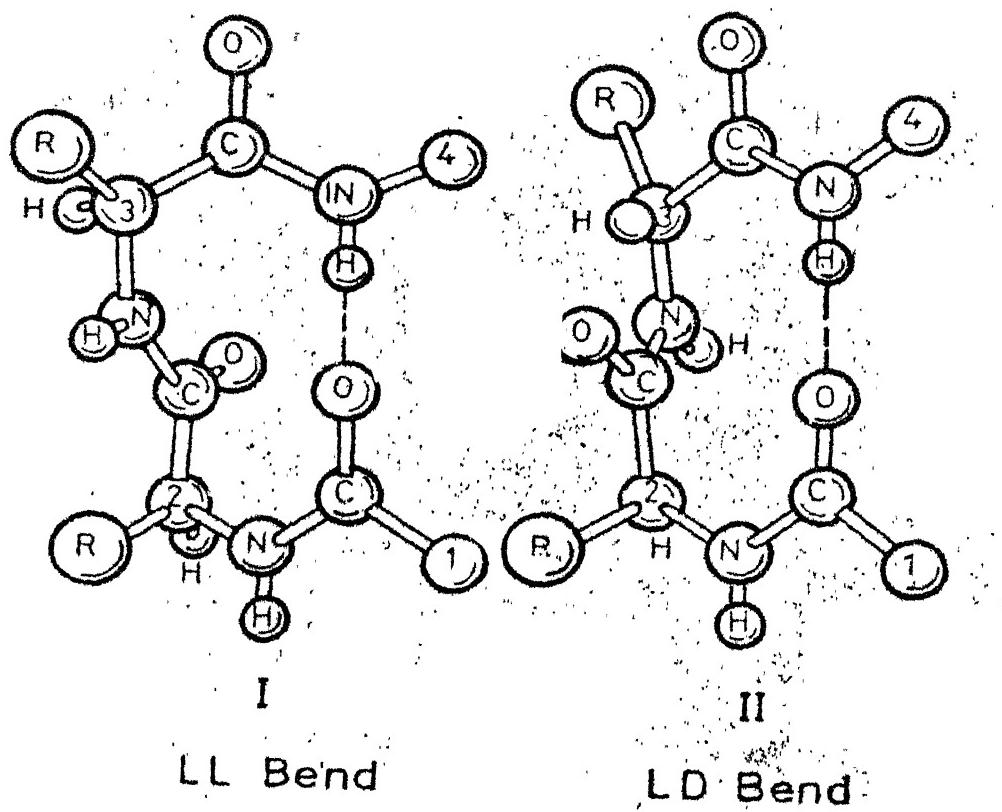


Fig.6

In fact, this theoretical prediction of Rao has been completely confirmed, by recent studies made on another peptide which have been published in a paper which appeared in Science of Nov.7, 1980 (19), and which I saw just one week before preparing this lecture. In this study, the β -turn (which will be discussed in the next section) that occurs in the lutenising hormone-releasing hormone (LH-RH) at X_2 and X_3 in its natural sequence -Tyr₁-Gly₂-Leu₃-Arg₄- was first shown to be stabilised and made more active by the introduction of a D-side chain at the Gly α -carbon atom. This agrees with ideas on the so-called Type II β -turns, which is explained below.. However, the same workers found that the activity of LH-RH is equally well improved by producing a γ -lactam ring using, however, the L-configuration at the Gly carbon atom for this purpose. The interesting point is, once again, that the β -carbon atom corresponds to the L-configuration at C $^{\alpha}$ for the γ -lactam ring, while it corresponds to the D-configuration for the linear peptide which showed increased activity. Once again we see that "L imitates D". This can be generalized, and it can equally well happen that D can imitate L under suitable circumstances in other compounds, especially those having the conformation of L-L β -turn (which is very common).

This may look very strange to you, but actually, it is easy to understand, when we realise that the (ϕ , ψ)-map throws away a large range of combinations of ϕ and ψ the moment there is a side chain that is free. This is because of a Van der Waals contact larger than 3 \AA that is required between non-bonded atoms.



When the β -turn was proposed from our laboratory (20) (which incidentally is of two main categories — Type I and Type II — both of which were pointed out by Venkatachalam and a Type III closely similar to Type I, but which forms part of the β_{10} -helix), it was realised that one of them (Type II) will not incorporate an L-amino acid in the third location of the sequence $-R_1-R_2-R_3-R_4-$, but only glycine can occur there normally. We had not realised at that time that D-amino acids occurred fairly commonly in antibiotics, although they occur very rarely in normal compounds taking part in biological metabolism. Therefore a couple of years later, Chandrasekaran and I worked on this so called L-L and L-D turns (standing for β -turns of type I and II) in Chicago. This (21) pointed out the great stability that the D-amino acid imposes on replacing Gly in Type II turns. The reason is very simple, namely that the D side group lends additional stabilizing energy in the region R_3 , (but an L C^β -atom destabilizes it). This again is a fact, which the paper I mentioned above on LH-RH has demonstrated so beautifully.

Table 2

(f) Side chains of amino acids

Since the side chain has played such an important part in the conformation of the backbone itself in peptide and protein chains, a very systematic study of all types of amino-acid side chain was taken up by Sasisekharan and a number of his colleagues, notably Lakshminarayanan and Ponnuswamy. These studies were

Table 2. Conformational Angles Phi and Psi for the Common Beta Turns^a

Type ^b	Nature of R_2 , R_3	(ϕ_2, ψ_2)	(ϕ_3, ψ_3)
I	$\underline{\underline{L}}$, $\underline{\underline{L}}$	$(-60^\circ, -30^\circ)$	$(-100^\circ, 10^\circ)$
II	$\underline{\underline{L}}$, $\underline{\underline{D}}$	$(-60^\circ, 120^\circ)$	$(80^\circ, 0^\circ)$
III	$\underline{\underline{L}}$, $\underline{\underline{L}}$	$(-50^\circ, -30^\circ)$	$(-50^\circ, -30^\circ)$
I'	$\underline{\underline{D}}$, $\underline{\underline{D}}$	$(60^\circ, 30^\circ)$	$(100^\circ, -10^\circ)$
II'	$\underline{\underline{D}}$, $\underline{\underline{L}}$	$(60^\circ, -120^\circ)$	$(-80^\circ, 0^\circ)$
III'	$\underline{\underline{D}}$, $\underline{\underline{D}}$	$(50^\circ, 30^\circ)$	$(50^\circ, 30^\circ)$

^a The hydrogen bond is 4 → 1 for all of them.

^b I', II', III' are mirror images of I, II, III, and therefore $\underline{\underline{L}}$ and $\underline{\underline{D}}$ are interchanged between the two.

started in the late 1960's (22) and almost all the 20 amino acids were studied. It was a great pleasure at the early stage of the subject for us to see which amino acid will have which side-chain conformation, and it was very reassuring when we found that not only were these confirmed by observation in small compounds, but even by the observed crystal structures of globular proteins.

Nowadays, data of this type is of common knowledge, and it is even contained in the Handbook of Biochemistry and Molecular Biology.

(g) Beginnings of energy calculations.

One of the very essential features that specifies which of two possible conformations, both of which are equally likely, will be preferred is the occurrence of hydrogen bonds — particularly of the types NH...O and OH...O. Therefore, in trying to calculate the energies, it is necessary to have a potential function for these. (I am not mentioning much about the early development of the energy calculations since our laboratory played only a secondary part in that feature. The first energy approaches to protein structures were given in the 1965 by Liquori (23), Flory (24) and Scheraga (25) almost simultaneously. We got into it almost immediately and preferred the Flory formulation of the potential functions which we applied for nonbonded interactions.) Here we used an approach which can be considered to be one belonging to scientific philosophy, namely, the application of statistics and probability to energies, and therefore I shall discuss it in some detail.

Statistical methods for conformational analysis

(a) Probability and energy of hydrogen bonds

Although this approach is widely used nowadays in several aspects — for example, for the prediction of secondary structure from sequence, as has been done by Gerry Fasman and Chou, (26) — it has not been sufficiently realised that earlier attempts at applying statistical methods for such purposes were made in our laboratory. In the early 1960's, along with Dr. C.Ramakrishnan who was the co-author of the first paper on (ϕ, ψ) -map, I investigated in great detail the distribution of the length $\underline{l}(\text{NH})$ and the angle $\theta = \text{NH}^\wedge \text{NO}$ in $\text{NH} \dots \text{O}$ hydrogen bonds. It was a very laborious work and we took almost all available data at that time and this was published in the Proceedings of a Symposium on Fibrous Proteins which took place in Canberra in Australia. Soon thereafter, we wanted to make use of this in predicting the energy distribution as a function $E(\underline{l}, \theta)$ of \underline{l} and θ from the probability distribution $p(\underline{l}, \theta)$ (27). For doing this, we used the Boltzman distribution:

$$p(\underline{l}, \theta) \propto e^{-E(\underline{l}, \theta)/RT} \quad (1)$$

This formula met with severe opposition because the Boltzman distribution has been proved and is utilised in physics only for energy distribution among molecules, or components of molecules which are in statistical equilibria. I had a long discussion with Professor Pauling about this when he came to Bangalore and I pointed out to him that the energy values so determined fitted beautifully into predictions of structures for biopolymers and

similar compounds. He was non-committal and said in effect; "If you find that it is empirically satisfactory, go ahead and use it". I have still not got the complete theory to support this distribution, although I have some vague ideas which I will not present here. The essence behind this is simply the fact that a conformation, which is expected to be rarely observed because of the higher energy involved, will in fact be rarely observed. The second "rarely observed" in the above sentence this refers to $p(\underline{l}, \theta)$ of Eq. (1) while the first "rarely observed" refers to the calculated energy $E(\underline{l}, \theta)$ of it. Any relation of the type of Eq. (1) will fit this; the only point at issue is whether the constant used should be RT or some other number.

In fact, this is a dictum of probability theory — namely that if a certain probability distribution is observed connecting one property with another property of a population, then the joint probability distribution can be equally well applied for predicting the second from the first, or the first from the second, in particular cases. Hence, it is obvious that the statistical method of approach can predict conformations only in a statistical way, and one should not be surprised if it gives completely wrong results in a particular case. If enough examples are tried, the fit will surely be good.

(b) Rarity of cis peptide units

This statistical approach for obtaining the energy distribution

function has been used in our laboratory in a number of ways. For instance, we know that the classical definition of the "partition function" in statistical mechanics which connects free energy with probability employs RT as the exponential parameter connecting the two. We used it, in particular, to explain the relatively rare occurrence of cis peptide units in relation to trans peptide units in protein and polypeptide chains, by using Eq. (1) in reverse. Although the difference in energy between these two states of a single peptide unit is only of the order of 2 to 3 kcal/mole the observation is that cis peptide units are extremely rare and are almost never found except for proline and for N-methyl-amino acids. A very elegant explanation of this was given by us in terms of the partition function obtained from the distribution of states in the (ϕ , ψ)-maps of a stretch of three peptide units (28). The calculations showed that, for the common amino acids with a C β -atom, the probability of a cis conformation in the middle peptide unit was extremely rare in relation to its having a trans conformation. However, for proline, the two were found to be practically of the same probability. This beautiful result has resolved what I had considered earlier to be one of the unsolved problems in peptide and polypeptide conformation. However, it does not mean that a cis peptide unit can never occur for residues other than proline; it can do so under special circumstances where the conformation of the chain and its local environment produces restrictions, requiring such a unit to be present. In other words, there is

no mystery about cis peptide units being rarely observed, except that it is a highly unlikely conformation for a three-peptide chain unconstrained by other considerations.

We also employed this statistical approach to determine the nature of the ϕ - and ψ -potential functions for amide units as they occur in a peptide chain, by actually looking at the distribution in the (ϕ, ψ) -map of various local conformations at the C^α -atom, and comparing it with the contribution expected from the intermolecular Van der Waals and repulsive interactions. It is rather surprising that the potential functions so obtained showed fairly steep maxima and minima for ψ with a barrier of more than 2 kcal/mole, as against a small value of less than 0.5 kcal/mole that had existed in the literature. It was also verified from carefully devised quantum chemical calculations that this type of variation is to be expected (see 29).

Application of quantum chemistry to peptide conformation:

This is the right opportunity to talk briefly about quantum chemistry and how it can help in conformational analysis. The above analysis of the ψ -potential and the associated quantum chemistry was done by my colleague Kolaskar with others in the department. Earlier, he was associated with Lakshminarayanan and me in studying the non-planarity of the peptide unit — a feature which we had pointed out to be of importance to biomolecular structure even in the 1968 review (30) in Advances in Protein Chemistry. Since then, several persons, including Dunitz in

particular, had analysed crystal structures from this point of view and showed that non-planarity was not at all uncommon. However, no definite indication was available from theory as to how much of non-planarity is to be expected and what is the energy associated with it.

(a) Catalysis of the theory of non-planarity

Our entering this field was catalyzed by a remark made by Prof. Mullikan commenting on my lecture, in a seminar that I gave on peptide conformation in Chicago. I greatly emphasized the importance of the planar peptide unit, and its dimensions as determined by Pauling, for the stereochemistry of peptides, and how it had helped in working out so many problems in peptide and protein conformations. Mullikan asked me, in particular, whether I believed that non-planarity cannot at all occur, and he suggested that the very fact that ammonia is pyramidal indicated that, even in the peptide unit having a partial double bond character for the C—N bond, the three bonds meeting at the nitrogen atom need not be completely planar. The very next week, Lakshminarayanan and I started making quantum chemical calculations to test this idea, because there was no other approach to it that could give a definitive answer. Using CNDO calculations, we showed that large non-planarity ($\Delta\omega$), of about 10° , can occur about the C—N bond, and the rotation angle ($\Delta\theta_N$) between the N—C^a and N—H can also differ from 180° by double this order of magnitude. Immediately, our attention was brought to a microwave

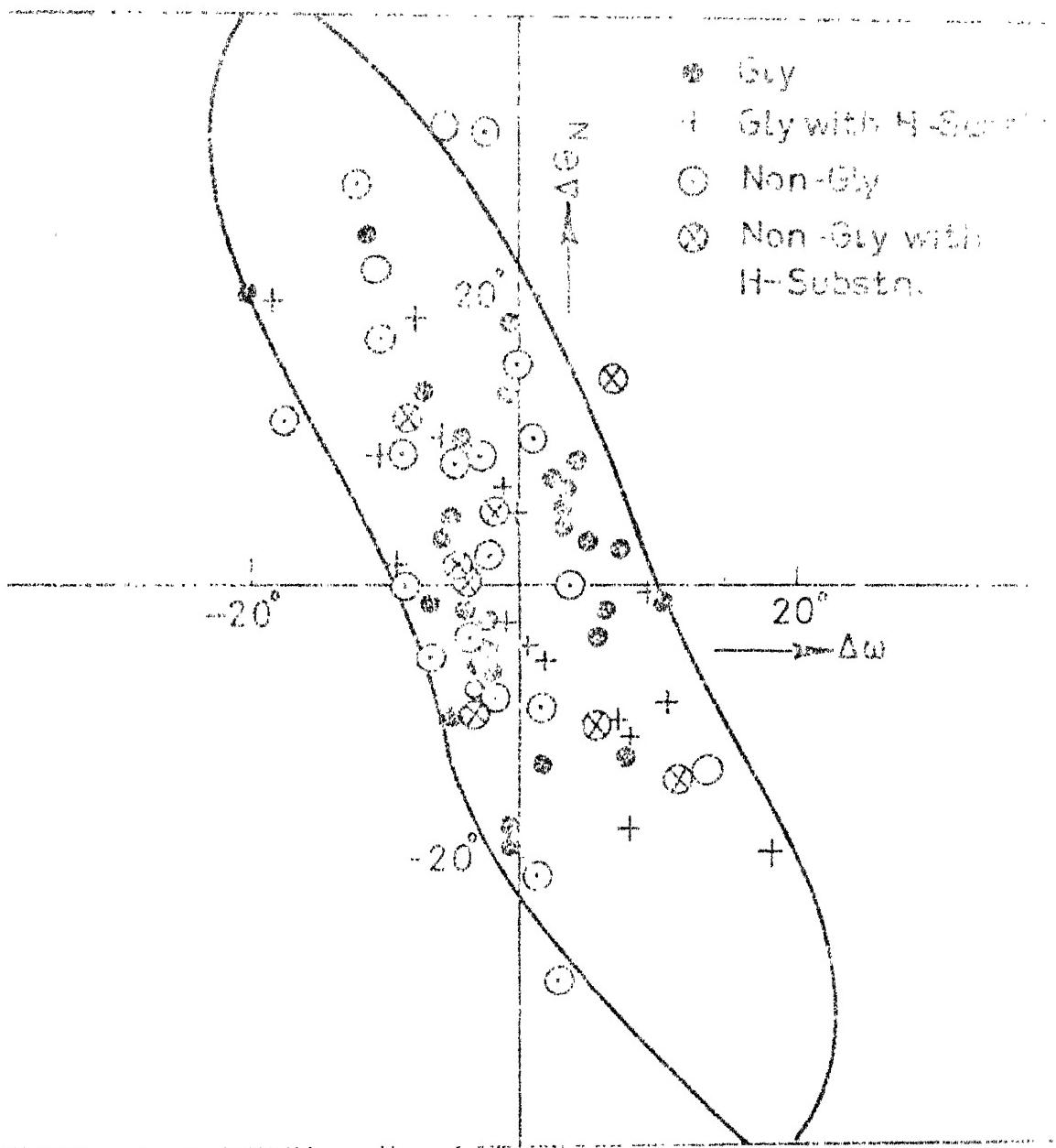
study made in Japan several years earlier on formamide ($\text{H}-\text{CO}-\text{NH}_2$), in which a nonplanarity of this order had been observed at N. It greatly strengthened our confidence in the result from quantum theory. However, when we applied INDO for this purpose, the predicted deviation was rather smaller, though still appreciable, and deviations from the planar structure of upto $10\text{-}15^\circ$ of non-planarity, at the N atom, did not involve increased energies of more than 0.5 kcal/mole. On the other hand, both CNDO and INDO indicated very little nonplanarity of the three bonds meeting at carbonyl carbon atom (31).

For a few years thereafter, Kolaskar spent considerable time in checking various available data and confirming, by the probability method mentioned above, not only that the distribution of non-planarity is what is given by theory, but also that the order of magnitude of energies involved was also in agreement with observation, if Eq. (1) is taken to be valid (See Fig. 8).

Fig.8. Energy map obtained from quantum chemistry (INDO) and observed data in good crystal structures of peptides.
(Symbols explained in text).

Non-planarity and its consequences for peptide conformation

This is the right occasion to talk of the application of the non-planar peptide unit in polypeptide structures. In the beginning, we found several examples in simple peptides and cyclic peptides, with appreciable non-planarity, as calculated



by using accurate data from crystal structures, in which there was no reason why the packing in the crystal should have lent a hand for the production of non-planarity. A slight non-planarity was found for the α -helix on energy minimization, which agreed that what Arnott had found by a refinement from x-ray diffraction data; but it was nothing to talk about. The general conclusion, of value to those who build protein structures, was that one need not worry about including non-planar peptide units with up to 20° non-planarity ($\Delta\theta_N$) at the nitrogen atom, and a range of about $\pm 10^\circ$ for the dihedral angle $\Delta\omega$ about the standard value of 180° for a trans peptide unit.

(a) Left-handed δ -helix with non-planarity

There the situation stayed until, by a curious coincidence, my attention was drawn to a possible left-handed helix of the α -type for a polypeptide chain. This was brought to my attention, at the NMR conference in Stanford, by Jardetsky as a probable conclusion of some of his NMR data. A brief inspection of the model he showed me indicated that this helix was of a topology different from the α -type helices. Although the ω -helix is left-handed, it has only $j \rightarrow 1$ hydrogen bonds, while in the helix built by Jardetsky it was $1 \rightarrow j$.

I told Jardetsky that we should be able to find, by calculation, the best helix having this topology. But, I also remarked that, only a year earlier, Ramakrishnan in our laboratory had made a thorough search of every possible type of

single helix that could occur for peptides, and had shown that all the possible ones had been listed and no new ones would be found if the currently accepted ideas of energy of stabilization were used. This was the dilemma; but then it occurred to me that the solution might lie in non-planarity. I was at the N.I.H at that time and had no assistants, and therefore I telephoned Chandrasekaran, who was at Purdue, and told him to find the minimum energy conformation in the region having this particular helicity, including also non-planarity. Surprisingly, Chandrasekaran then found a good minimum in the expected region of Jardetsky's left-handed helix, for poly-L-alanine. Although it was not as stable as the right-handed α -helix, it was probably superior to all the left-handed helices of the type that were considered to be possible, like α_L and ω .

Therefore, I examined other polypeptides as likely candidates for this new left-handed helix with about -4.0 residues per turn. Earlier, in Madras, we had found that poly-L-serine could form an OH...O hydrogen bond between the side chain $-C^{\beta}H_2-OH$ and the backbone $O=C$, if it had a left-handed helical twist of the usual α -type. On checking the same polypeptide for the new left-handed helix, I found that a similar hydrogen bond could exist for this also. If this were true, then this would also be true for the side chain $-C^{\beta}H_2-NH_2$. The corresponding polypeptide is poly-PDPA (standing for poly-L-diamino-propionic acid). This is an analogue of lysine and ornithine,

with one less CH_2 group than ornithine. On checking with models, I found that both lysine and ornithine were not specially suited for the new helix, but the side chain of PDPA was very good for forming a hydrogen bond with the backbone.

I left it at that; but imagine my surprise, when in 1978, at the annual Biophysical Society Conference in Washington, J.T. Yang of San Francisco, to whom I talked about this, told me that he had already discovered that L-PDPA had a left-handed helix, while both poly-L-lysine and poly-L-ornithine assumed only the right-handed helical configuration, as detected by ORD-CD studies. I was then absolutely convinced that our ideas about the new left-handed helix were right, and we decided to name this as the δ -helix. A paper was published on the theoretical study, and possible interpretations of NMR and ORD-CD data employing this helix, by Chandrasekaran and Jardetsky (8).

We can now show that the δ -helix is the stablest of all left-handed polypeptide helices. In fact, my former colleague Manju Bansal, told me two weeks before preparing this lecture, that she had definitely established that the helix which occurs for poly- β -benzyl-L-aspartate (PBLA) is the new δ -helix having $n = -4.0$ and not the ω -helix which is usually supposed to occur (9). The proof from theory was obtained by taking into account especially the potential energy associated with non-planarity of the peptide units, and also the various improvements in the potential functions which I mentioned above,

including, in particular, the idea of softening the contacts H...H and C...H which I had suggested in my contribution to the Jerusalem symposium in 1975 (29). We can now exclude the ω -helix from the list of possible helices since its minimum energy for PBLA is about 10 kcal/mole above that of the δ -helix. (So it has not been listed in Table 1). All examples where the former had been postulated should be checked for fit with the new δ -structure.

Need for looking out for unexamined possibilities:

The above is a very good example where, an entirely new possibility could be found out, although a thorough re-examination of the available data and theory indicated that no new polypeptide helix was expected to occur at all. Thus, from the point of view of scientific philosophy, one must have one's eyes and ears open for new type of knowledge leading to new possibilities, even though they are completely at variance from accepted theory. As the famous Indian poet Kālidāsa mentions:

Purāṇamityeva na sādhu sarvam
Na cāpi kāvyam navamityavidyam.

(Not all that is old is necessarily true;
Nor a poem be unread, because it is new.)

This shows that this problem has been there all along in human existence, and will continue to exist. The bright young man has always to fight the established order, before his new ideas are accepted.

(a) The Nucleic Acid Dilemma.

I shall therefore briefly consider what has happened similarly in the case of the DNA double helix. The postulation of the double helix in 1952 by Watson and Crick from stereochemical and base-pairing principles was proved by the work done in King's college in the succeeding years. The x-ray patterns of many polynucleotides agree with that of the DNA double helix. Apart from the existence of minor modifications such as A-DNA and B-DNA which had different number of units per turn, both of which had essentially the same right-handed twist of about 30-40° and base pairing of the Watson-Crick type, only minor examples had been found where slightly different configurations existed. However, whenever I talked to biologists during the late 60's and early 70's, when so many experimental studies had been made on DNA as it occurs in the nucleus of the cell, they always had a difficulty in reconciling the way in which a nucleic acid chain will have to untwist itself some millions of times in one molecule of DNA and then, after duplication, retwist itself in the same way without any tangling taking place, with the absolute reproducibility of genetic information achieved by this process. I was also worried very much about this feature, and frequently talked about this to experts in DNA conformational theory — particularly with Sasisekharan of our laboratory. Independently, Sasisekharan and himself thought about the possible existence of left-handed helices for DNA and had stereochemical calculations showing that it had a very

reasonable structure and could possibly occur. However, this matter was under eternal discussion between biochemists, microbiologists, molecular biologists, and molecular biophysicists, and no clear solution to the tangling problem was available.

During 1975-76 I took a serious interest in this, and thought that the matter could be resolved by putting the two chains of DNA side by side, but having some sort of wavy structure so that the helical x-ray pattern would be simulated. In fact, I even went to the extent of making some drawings of the chain that would have the same repeat as normal DNA, and calculated the expected diffraction pattern, using one lumped atom at phosphorus, another at the sugar, and the third at the base. The model was extremely crude and was of the 1950 era. But the interesting thing was that the calculated Fourier transforms were compatible with the observed pattern, as judged by discrimination between regions of large intensity and those of small intensity. All these only showed that the net radius, or the net width, of the structure was correct and that the two chains had some sort of helicity with the same pattern as in DNA.

However, the whole approach had to be thrown away because Sasisekharan showed unmistakably that such an arrangement cannot be realised in an actual DNA structure. He was sure that, if we assume that the two chains do not twist around one another but only stay side by side, then no such structure can be built which is free of bad contacts. In fact, I would consider this a very great achievement for a nucleic acid expert, because I

myself was completely baffled by the number of dihedral angles that are there in DNA, and the number of inter-connections that had to be considered. To say with confidence that something is not possible required a very great feeling for the molecular structure.

(b) The Zig-zag Structure of Sasisekharan

Taking his clue from these discussions in the department, which raised the question whether the intertwisting of the two chains in DNA is a biological possibility (quite apart from the chemical possibility in the specimens which give the beautiful diffraction patterns recorded for crystallised B-DNA), Sasisekharan then tried to fit a structure, in which, the structure is right-handed for about 5 units, and is then left-handed for about 5 units, so that there is a repeat after about 10 units as is found in B-DNA. Here again, an enormous amount of intuition and knowledge of how these structures would look like was necessary in order to show that something is possible from stereochemistry. When I tell you that, even if some of the dihedral angles and bond angles were changed by $\frac{1}{2}^\circ$, the net unit twist would go away by a magnitude of the order of 20° , one can realise the complexity of the problem. Yet, Sasisekharan showed that such a structure is quite satisfactory, and much of it was made possible because he already had the coordinates for the left-handed DNA helix. He published this work first in Current Science (32) and later in the Proceedings of the US National

Academy of Sciences (33). This alternating structure (now called the zig-zag structure) is very attractive to the biologist, as he does not have to bother about the very large number of un-twisting rotations which DNA has to undergo during the process of replication. (I do know that, if nicking and sealing take place, then this need is not there.)

As you all know, the matter stood at that, and it took some time before some of these structure were actually realised in examples where they could be unmistakably shown to occur. Thus a short stretch of left-handed helix was observed in oligo-nucleotides by Viswamitra in 1978 (34), by Rich in 1979 (35) and by Dickerson in 1980 (36). Mainly as a result of this support of experiment to theory, the theoretical results worked out by Sasisekharan and his co-workers have now assumed great importance, and his approach can be used for building various possible types of structures for polynucleotide.

I will not say more about this, mainly because I am not a specialist on polynucleotides and the above comments of mine have been made only as a biopolymer chemist viewing the subject as a whole. A recent review by Sasisekharan (37) contains references to the relevant literature.

Suggestions for Future Studies

I shall now give a brief account of some ideas that I have regarding types of problems in biochemistry and molecular biology, which could be attacked profitably from the point of view

of conformation. They are, by no means, exhaustive.

(a) Molecular Fit

The concept of "molecular fit" occurs, for example, in the binding of the substrate to an enzyme. A very similar problem is that of antigen-antibody recognition. As Pauling and Delbrück (38) pointed out as early as 1940, the essence of the phenomenon is the pairing of a specific arrangement of atoms in one molecular with that in the other molecule which comes and attaches itself to it.

On the factual side, the common three-dimensional architecture of the reactive groups occurring in the active sites of related enzymes has been sorted out from x-ray crystallographic data (for example, by Rossman (39)). The time is now ripe for the theorists to tackle this problem and to make energy calculations on the recognition of particular molecular species, or atomic arrangements, by enzymes.

(b) Recognition by antibodies

That this is not too difficult, and that some apparently contradictory facts can be given a sound explanation from a proper understanding of conformational theory, has been shown in the case of antigen-antibody specificity in a recent work done in Bangalore by Rao and co-workers (40). It is commonly supposed that, in the saccharide chain of an antibody, it is the terminal sugar residue that gives much of its specificity. However, in the case of two such compounds, lacto-N-neotetraose (a)

and lacto-N-tetraose (b), both of which have the same end group, galactose, the former has the specificity for binding, while the latter does not bind at all. The only difference between the two is that the former has an $1 \rightarrow 4$ linkage of galactose to N-acetyl-glucosamine, while it is $1 \rightarrow 3$ in the latter between the same two sugars. However, if one adds an L-fucose residue to the second compound with a $1 \rightarrow 2$ linkage to obtain lacto-N-fucopentaose, then a good amount of the binding is restored. These are known facts, which look puzzling. However, considering that not only the terminal residue, but two or three others next to it in the chain, are also responsible for recognition and binding, Rao showed that if the proper energy-minimised conformation of the above three compounds are compared, then the shape, as far as binding is concerned, is very similar as between (a) and (c), but different in the case of (b). This is shown in Fig. 9, and this is an example where a careful study of the relevant saccharide conformation helps in understanding the apparently strange behaviour that is observed.

Hence, a detailed study of the conformation of oligosaccharides, of widely varied types containing upto 5 or 6 residues, is called for. Nathan Sharon has estimated that even if 5 or 6 residues containing the various known sugars are considered, but the different types of linkages are taken into account, then more than a million varieties of conformation can be visualized. Thus, the reason why polysaccharides are so commonly associated with antibodies, blood groups etc., becomes understandable.

Fig.9. Schematic representation of compounds (a), (b) and (c) (see text), in relation to the binding pockets in the receptor. Note how the Gal in (b) is pointed away, while the additional L-Fuc in (c) restores the situation as in (a).

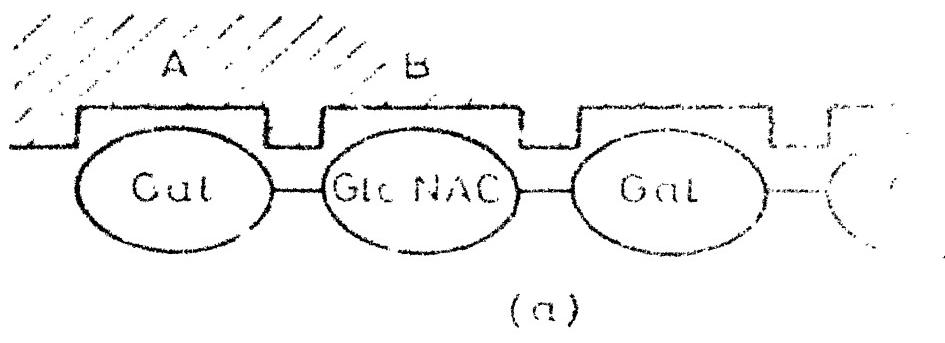
(c) Protein-Nucleic Acid Interactions

This is a subject in which there are more expert specialists than I taking part in this conference, and so I shall only touch upon it. The importance of intercalation within the nucleic acid chain, preventing its normal structure from being formed, is well recognized, particularly in relation to certain types of antibiotics and carcinogenic compounds. However, precise knowledge as to how a peptide unit, or its side chain, fits into a nucleic acid chain is not yet available, nor even the principles connected with the stereochemistry of it. In this connection, I would like to draw your attention to a recent paper by Visvamitra (41) on the x-ray crystallographic study of the synthetic analog, TANDEM, of the antibiotic drug triostin A, using the data of which, the first detailed picture of the association of a cyclic peptide with the DNA chain having a specific sequence has been worked out — see Fig. 10.

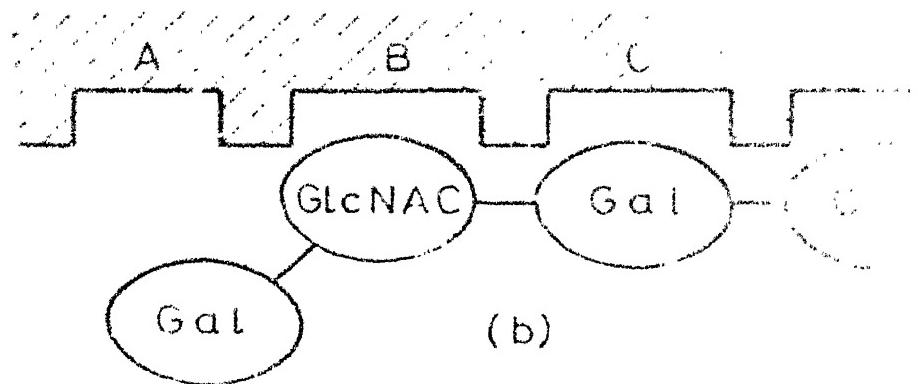
Fig.10. (a) CPK model of TANDEM molecule, slightly modified from the x-ray structure.
(b) Similar model of its complex with a partially unwound B-DNA helix, seen from the major groove side.

(d) Stereodynamics

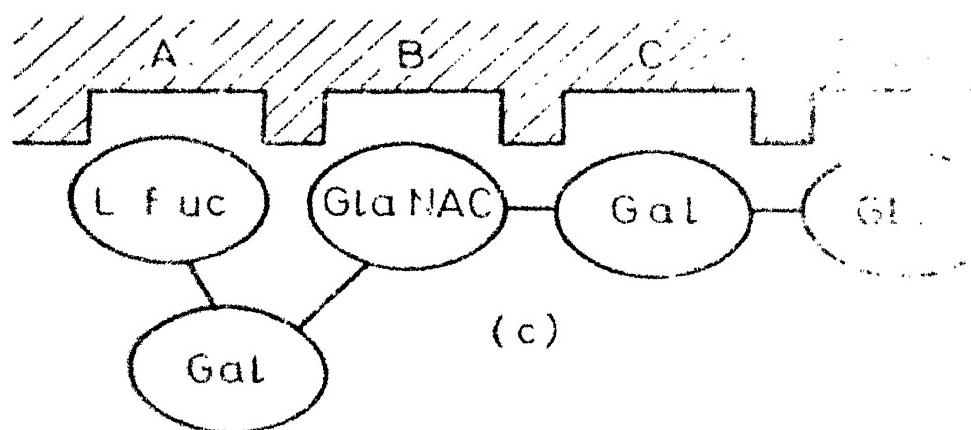
Finally, I come to the topic which is particularly empha-



(a)



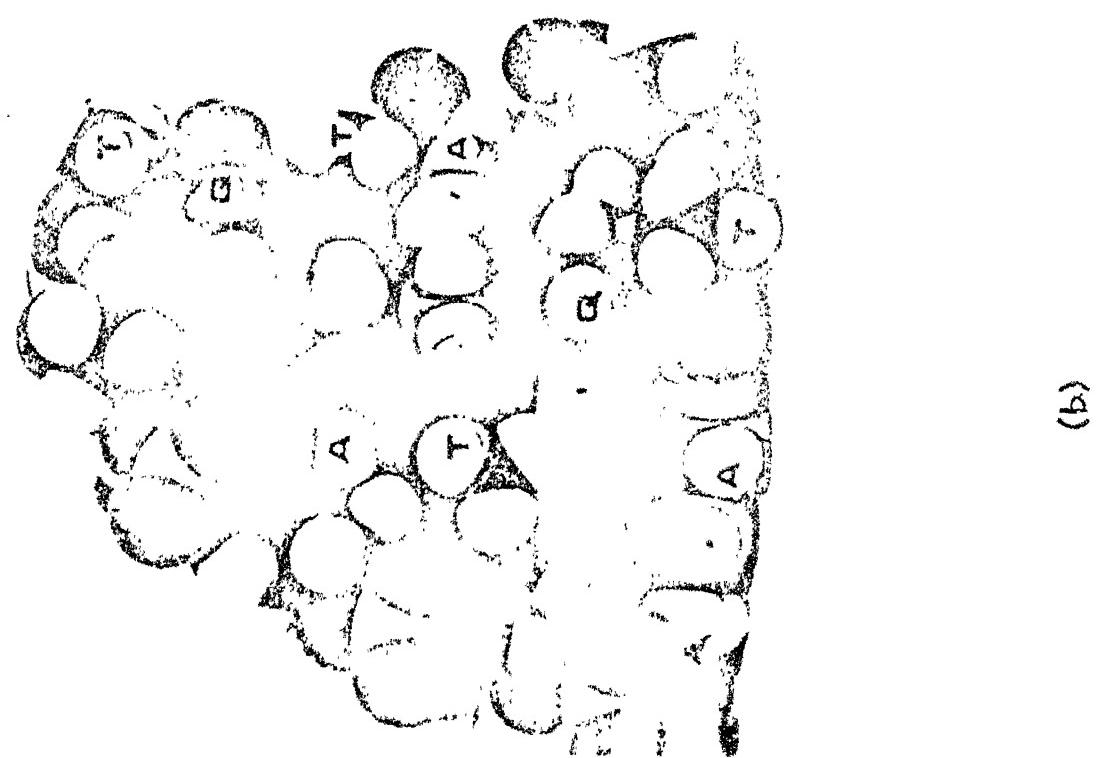
(b)



(c)



(a)



(b)

sized in this symposium — namely the stereodynamics of molecules. Dynamics is more difficult to work out than statics. However, efforts by Karplus and others in this direction have been very rewarding. I may point out two particular aspects where the dynamic action has to be studied in particular. One would be the way in which the active site of an enzyme moves over the surface, or the chain, of a biopolymer (like a protein) and reaches the particular specific sequence where the cleavage, or some other reaction, takes place. There is reason to believe that the recognition is there, not only of the actual substrate region where the reaction takes place, but also of the amino acids on either side upto 3 or 4 residues away. The dynamics of the "crawling" motion has to be understood, in addition to the phenomenon of "matching".

Similarly, the problem of ion transport across membranes, and its modification by ion transport peptides, is a very important problem to be examined. Thus, molecules like gramicidin-A, have a special type of helix — the so-called LD helix — first worked out by Chandrasekaran and myself (42, 43), although I have not touched upon this in this review. This helix has a central hole through which the ions are transported. However, the ion has to be of the right size — neither too small nor too large. If it is too large, obviously it cannot be transported through the hole, while if it is too small, it just goes in and comes out. When it is of the right size, one section of the tube takes hold of the ion, and moves it on to

the next section, apparently in some sort of peristaltic process. The dynamics of this, and the way whereby the amount of transport, normally taking place across the membrane, is enormously magnified by the peptide, should be examined. This will have the reward that it might be possible to design newer and better antibiotics of the gramicidin-A type.

Similarly, the other type of ion-transport antibiotics of the alamethicin type (such as suzukacillin, emerimycin, antimoebins, trichotoxin, and hypelcins) all contain the unusual amino acid α -aminoisobutyric acid (Aib), which is non-asymmetric, in that it has two $-C^{\beta}H_2$ groups attached to the C^{α} -atom. The conformation of peptide sequences of this unusual amino acid has been studied in great detail by Balaram and his group in Bangalore (for references see 44, 45). The main result is that it can have only highly restricted (ϕ , ψ)-values, and that it readily forms the 3_{10} -helix, by making Type III β -turns. Since this helix is not large enough to contain an ion inside, the ion-transport induced by it is cooperative, and some 5 or 6 chains probably take part in it, and there is practically no selectivity. The stereodynamics of this large molecule in the milieu of the membrane deserves careful study.

(e) Need for Elementary Book on Conformation.

This brings me to the last topic, namely the need for more elementary books on conformation specially intended for the biochemists and the biologists, who would like to employ for their studies, the methods of reasoning adopted by physical

chemists and chemical physicists. Since it is a way of thinking that has to be passed on to the biochemist and the biologist, and not merely a technique, there is a great need for books written on conformation where the emphasis is on the role of conformation related to biomolecules and biological activity, rather than on the principles of calculating energies and physico-chemical factors. Even the beautiful book by Dickerson and Geis.(46) has to be supplemented by another which will also explain the theoretical approach to the subject, in addition to the "what" and "how" of it that has been beautifully pictured and explained therein.

As in every science, conformational analysis has started as a speciality, and developed as a speciality; but I think it has now come to a stage when it can be made available to one and all.

Acknowledgements

Most of the material in this review was dictated from memory, and I beg to be excused for minor inaccuracies in the text, although I hope there are no serious errors. I wish to thank M. Suresh, M.V. Manjula and R. Manjunath, for typing several drafts of this report in less than three weeks, and for helping in the preparation of figures, tables etc. This work was done during the tenure of a research grant on "Application of Epistemology to Mathematics, Physics and Biology", provided by the University Grants Commission, India.

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MATRIX ALGEBRA FOR SENTENTIAL LOGIC

AND THE FORTRAN PROGRAM

MATLOG

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1. Introduction

In MATPHIL Reports No. 12, [1], we had given a detailed picture of how a FORTRAN program can be worked out for logical operators and how the logical analysis of an argument in Propositional Calculus can be done in terms of these operators. Earlier, in MATPHIL Reports No. 8 [2], the principles of the technique, which has been given the name NYAYA, were explained with reference to the general problem of computerising logic. In this report, we shall consider a variation of the approach adopted in NYAYA, namely the use of matrix formalism, called MATLOG, which appears to be much more convenient for being extended to other aspects of logic such as Quantified Predicate Logic. Thus, by using 2×2 Boolean matrices for all classical logical operators such as "equivalence", "negation", "and", "or", "if", "nand", "nor" etc., and slightly modified forms of these for the purely SNS operators "agree", "with" and "upon", all types of logical relations in propositional calculus can be implemented in this

formalism.

As described in the earlier papers, all these require the introduction of two more states $\underline{\underline{D}}$ and $\underline{\underline{X}}$, in addition to the classical states \underline{T} and \underline{F} which are well-known, for a logical term. We have also shown that these four states can be expressed by two-element Boolean vectors of the type $(\underline{a}_\alpha \quad \underline{a}_\beta)$ which have the four states $(1 \quad 0)$ for \underline{T} , $(0 \quad 1)$ for \underline{F} , $(1 \quad 1)$ for $\underline{\underline{D}}$ (the "doubtful" state) and $(0 \quad 0)$ for $\underline{\underline{X}}$ (the "impossible" state).

When we wish to find the relation between the state of a vector \underline{a} and that of another vector \underline{b} , since each of them can be represented by two-element Boolean vectors, the relation naturally be represented by a 2×2 Boolean matrix. This is the essence of the matrix algebra which is developed here.

typical example, the truth table for the operator "and" in Table 1(a). The four truth states that are shown in the body of the Table 1(a) are converted into a matrix $|\underline{A}|$ in the form shown in Table 1(b), by using the code " $\underline{T} = 1$ " and

Table 1

(a) Truth Table for "and"

<u>a</u>	<u>b</u>	T	F
T	T	T	F
F	F	F	F

(b) 2 x 2 Matrix for "and"

$$|\underline{A}| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

This straightforward method of converting the logical truth table of a binary relation into its corresponding matrix is completely general in MATLOG, and is used for generating all the classical operators. (More details can be seen in Ch.3 of [3].)

Thus, if we use the truth tables for N (not) we obtain its matrix as

$$|\underline{N}| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (1a)$$

Then the unary relation a N = b has the counterpart (1b) in matrix notation, using bra-vectors, $\langle \underline{a} |$ and $\langle \underline{b} |$, to represent a and b, and the matrix $|\underline{N}|$ to represent the relation N :

$$\langle \underline{a} | \underline{N} | = \langle \underline{b} | \quad (1b)$$

This leads from Eq. (1) to the two results in (2a) and (2b) which give the logical consequences of the relation (1b) :

$$(1 \ 0) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (0 \ 1) \text{ or } \underline{a}_T \rightarrow \underline{b}_F \quad (2a)$$

and

$$(0 \quad 1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (1 \quad 0) \text{ or } \underline{a}_F \mapsto \underline{b}_T \quad (2b)$$

When it comes to binary operators, the formulae are slightly more complicated. It can be shown from the general theory of relations (see [3]), that for the binary relation $\underline{\underline{a}} \underset{\sim}{Z} \underline{\underline{b}} = \underline{\underline{c}}$, the two components \underline{c}_α and \underline{c}_β of $\langle \underline{\underline{c}} \rangle$ are given, in terms of $\langle \underline{\underline{a}} \rangle$ and $\langle \underline{\underline{b}} \rangle$, by the equations :

$$\langle \underline{\underline{a}} | \underline{\underline{Z}} | \underline{\underline{b}} \rangle = \underline{c}_\alpha \quad (3a)$$

$$\langle \underline{\underline{a}} | \underline{\underline{Z}}^C | \underline{\underline{b}} \rangle = \underline{c}_\beta \quad (3b)$$

where $|\underline{\underline{Z}}|$ is the 2×2 matrix corresponding to the operator $\underline{\underline{Z}}$, and $|\underline{\underline{Z}}^C|$ is obtained by complementing all the Boolean elements of $|\underline{\underline{Z}}|$. Thus, the state of the term $\underline{\underline{c}}$ in the form $(\underline{c}_\alpha \quad \underline{c}_\beta)$ can be immediately obtained when the states of $\underline{\underline{a}}$ and $\underline{\underline{b}}$ are given in the form $(\underline{a}_\alpha \quad \underline{a}_\beta)$ and $(\underline{b}_\alpha \quad \underline{b}_\beta)$, using only vector-matrix algebra. It should be emphasized that the Dirac products in Eqs. (3a) and (3b) involve only Boolean multiplication and addition. In fact, throughout this report, we shall use only Boolean algebra both for addition and multiplication, which are then applied to matrix operations like vector-vector products, vector-

matrix products and matrix-vector products.

In effect, if equations of the type of Eqs. (1b), and (3a) and (3b), can be worked out, then we can evaluate the effect of any unary logical connective or a binary logical connective. Since, we can show (see Ref.3) that any argument in sentential logic can be ultimately decomposed into unary relations and/or binary relations arranged in sequence, it follows that the implementation of the above two types of equations will be sufficient for analysing any general logical argument (see later for "reverse" relations and their representation in matrix algebra).

In this report, we shall not discuss the basic theory, although we will consider how the matrix-algebraic formulae can be used for working out the sequence of operations in an argument. The main emphasis will be on the implementation of the technique in FORTRAN, to obtain the program MATLOG. The proofs of the theorems and formulae used here can be found in Ref.3. However the discussion here will be made sufficiently self-contained, by

listing the properties of the various operators that are relevant.

Also, the way in which they are put together and implemented will also be explained, by discussing examples where they are applied.

It should be emphasized that, unlike NYAYA, which has an exact counterpart in terms of electronic logical circuits in the analog computer ESNY [4], the algebra of MATLOG is arithmetical in content, and is best implemented in a standard digital computer, and hence it is that the FORTRAN implementation of this is particularly described in this report.

2. Truth values, variables and matrix operators.

(a) Truth values

As in the case of NYAYA, in MATLOG also the states of a logical term are four in number, namely —

$$(1 \quad 0) = \underline{\underline{T}}, \quad (0 \quad 1) = \underline{\underline{F}}, \quad (1 \quad 1) = \underline{\underline{D}}, \quad (0 \quad 0) = \underline{\underline{X}} \quad (4)$$

with the same significance as before. Thus, the two possible states of any statement, namely truth and falsity, are represented

by the two "pure" states $(1 \quad 0)$ and $(0 \quad 1)$. For this reason,

the symbol $\underline{\underline{P}}$ is used to represent $\underline{\underline{T}}$, or $\underline{\underline{F}}$, when it is unique.

Then, we have the "mixed" state $\underline{\underline{D}}$, which is the state for which

one does not get a definite answer "yes" uniquely for either $\underline{\underline{T}}$

or $\underline{\underline{F}}$, but both answers (either $\underline{\underline{T}}$ or $\underline{\underline{F}}$) are possible, so that we

call it the "doubtful" state. In the sense of the Boolean addi-

tion symbol \oplus ,

$$\underline{\underline{D}} = (1 \quad 1) = (1 \quad 0) \oplus (0 \quad 1) = \underline{\underline{T}} \oplus \underline{\underline{F}} \quad (5)$$

On the other hand, the so-called "impossible" state $\underline{\underline{X}}$ corresponds

to the simultaneous existence of $\underline{\underline{T}}$ and $\underline{\underline{F}}$, which is contradictory,

and therefore it can be represented, as in (6), using the symbol

\otimes for Boolean multiplication :

$$\underline{\underline{X}} = (0 \quad 0) = (1 \quad 0) \otimes (0 \quad 1) = \underline{\underline{T}} \otimes \underline{\underline{F}} \quad (6)$$

We shall use the same meanings for the Boolean additive and

multiplicative symbols \oplus and \otimes , as in NYAYA, namely as stand-

ing for the operators \underline{U} and \underline{W} already introduced.

(b) Connectives

(i) Unary operators:

The real difference between the programs NYAYA and MATLOG lies in the representation of the connectives between states representing two different terms, or three different terms, which have logical relations between them. We do not use logical operators like AND, OR, NOT etc for this purpose, but matrix operators which pre- or post-multiply the state vectors. Thus, from the theory of relations, we use the result that if \underline{a} is related to \underline{b} by a "relation" \underline{Z} , in the form $\underline{a} \underline{Z} \underline{b}$ then it is represented in the matrix form by the equation :

$$\langle \underline{a} | \underline{Z} | = \langle \underline{b} | \quad (7)$$

In the case of logic, where the terms \underline{a} and \underline{b} are represented by 2-element Boolean vectors, $|\underline{Z}|$ is a 2×2 Boolean matrix. Thus, in general, unary relations can be represented in the form of Eq. (7), and the particular cases of the classical connectives E and N may be illustrated by Eqs. (8) and (9).

$$\langle \underline{a} | \underline{E} | = (\underline{a}_\alpha \quad \underline{a}_\beta) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = (\underline{b}_\alpha \quad \underline{b}_\beta) = \langle \underline{b} | \quad (8)$$

$$\langle \underline{a} | \underline{N} | = (\underline{a}_\alpha \quad \underline{a}_\beta) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (\underline{b}_\alpha \quad \underline{b}_\beta) = \langle \underline{b} | \quad (9)$$

Obviously, they have all the properties expected of the connectives "equivalence", and "negation". It is to be particularly noted that the negation operator $\underline{\sim}$, in addition to interchanging the \underline{T} and \underline{F} states, as between \underline{a} and \underline{b} , leaves invariant the states \underline{D} and \underline{X} . Thus,

$$(1 \quad 1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (1 \quad 1) \rightarrow \underline{a}_D \underline{\sim} = \underline{b}_D \quad (10a)$$

$$\text{and } (0 \quad 0) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (0 \quad 0) \rightarrow \underline{a}_X \underline{\sim} = \underline{b}_X \quad (10b)$$

We may similarly consider the unary operator \underline{Y} for imply, which is represented by the matrix

$$|\underline{Y}| = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \quad (11a)$$

It is readily seen that the corresponding relation between \underline{a} and \underline{b} in

$$\langle \underline{a} | \underline{Y} | = \langle \underline{b} | \quad (11b)$$

which leads to the logical consequences

$$\underline{a}_T \rightarrow \underline{b}_T , \quad \underline{a}_F \rightarrow \underline{b}_D \quad (11c)$$

which have been discussed in detail in [3]. It is obvious that there can be only $2^4 = 16$ possible different operators having this property of being representable by a 2×2 Boolean matrix. We shall discuss the nature of these and list them in the next section.

However, we may mention the very interesting possibility of representing the "reverse" of a unary relation very simply by transposing the matrix. Thus,

$$\langle \underline{a} | \underline{z} | = \langle \underline{b} | \iff \langle \underline{b} | \underline{z}^t | = \langle \underline{a} | \quad (12)$$

which is an immediate consequence from the general theory of relations (see [3]). As an example, if $\langle \underline{a} | \underline{y} | = \langle \underline{b} |$ represents "a implies b", then $\langle \underline{b} | \underline{y}^t | = \langle \underline{a} |$ represents "b implicates a", for which we have the symbology $\langle \underline{b} | \underline{v} | = \langle \underline{a} |$.

This possibility of representing "reverse" unary operators by transposed matrices is extremely useful for "reversing" the

path in a general argument when necessary.

(ii) Binary operators:

The logical relation $\underline{a} \underset{\sim}{\wedge} \underline{b} = \underline{c}$, can be represented in the vector-matrix formalism that is adopted in MATLOG in the following manner [3]. Obviously the two terms \underline{a} and \underline{b} , when related by the connective $\underset{\sim}{\wedge}$, become equivalent to a new term \underline{c} ; and our attempt is to find the state of \underline{c} among one of the four SNS states, given the states of \underline{a} and \underline{b} . The formulae for this turn out to be very simple. If the connective $\underset{\sim}{\wedge}$ is represented by the matrix $|\underline{Z}|$, then

$$\langle \underline{a} | \underline{Z} | \underline{b} \rangle = \underline{c}_\alpha \quad (13a)$$

and

$$\langle \underline{a} | \underline{Z}^C | \underline{b} \rangle = \underline{c}_\beta \quad (13b)$$

where $(\underline{c}_\alpha \quad \underline{c}_\beta) = \underline{c}$ (14a)

and $|\underline{Z}^C| = \text{complement of } |\underline{Z}| = |\underline{Z}|\underline{M}|$ (14b)

In this, the complement of a matrix is obtained by substituting each element in the matrix by its Boolean complement — i.e.

0 by 1, and 1 by 0. Although this process is not representable by a matrix operation, we shall represent it, for the sake of uniformity, by the symbol $|\underline{M}|$ as shown in (14b). Typical examples of such complementations are

$$|\underline{E}^c| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} |\underline{M}| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |\underline{N}| \quad (15a)$$

$$|\underline{A}^c| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} |\underline{M}| = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} = |\underline{N}| \underline{O} |\underline{N}| \quad (15b)$$

We have found it very convenient to separate the 16 possible 2×2 matrices into 8 pairs, each pair being related by the operation of complementation of the matrix. These are listed in Table 2.

(c) FORTRAN representation of truth values, variables and matrix operators

(i) Truth values:

As already mentioned, there are 4 states \underline{T} , \underline{F} , \underline{D} , \underline{X} and these are represented by the symbols MSTR, MSFL, MSDF, MSXX, where M is added in the beginning to distinguish the corresponding quantity in MATLOG from that in NYAYA. Under MSTR, MSFL, MSDF, MSXX are

Table 2. 16 Matrices and their components

Logic	Name FORTRAN	Matrix	K1	K2	K3	K4
E	MZEE	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	1	0	0	1
E ^c (N)	MZEM	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	0	1	1	0
A	MZAE	$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$	1	0	0	0
A ^c	MZAM	$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$	0	1	1	1
Y	MZYM	$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$	0	1	0	0
Y	MZYE	$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$	1	0	1	1
V	MZVM	$\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$	0	0	1	0
V	MZVE	$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$	1	1	0	1
O	MZOM	$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$	0	0	0	1
O	MZOE	$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$	1	1	1	0
R	MZRE	$\begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}$	1	1	0	0
R ^c	MZRM	$\begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}$	0	0	1	1
C	MZCE	$\begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}$	1	0	1	0
C ^c	MZCM	$\begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}$	0	1	0	1
D	MZDE	$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$	1	1	1	1
D ^c	MZDM	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$	0	0	0	0

Footnote to Table 2.

The full names of the 16 Boolean 2 x 2 matrix operators are as follows :

MZEE = Equivalent.

MZEM = Negation.

MZAE = And.

MZAM = Nand.

MZYM = Does not imply.

MZYI = Implies.

MZVM = Does not implicate.

MZVE = Implicates.

MZOM = Nor.

MZOI = Or.

MZRE = "Row true", a is true irrespective of b.

MZRM = "Row not true", a is false irrespective of b.

MZCE = "Column true", b is true, irrespective of a.

MZCM = "Column not true", b is false, irrespective of a.

MZDE = "Universal Doubt", a is disconnected with b.

MZDM = "Impossible", a is contradictory to b.

stored the character constants 'T', 'F', 'D', 'X'.

(ii) Variables:

The corresponding variables in MATLOG are of the form MVA, MVB, MVC etc. and each of them can take any one of the four states MSTR, MSFL, MSDF and MSXX.

For manipulation by matrix multiplication, any variable is represented by a 2-element vector. For example, the α - and β -components of MVA are denoted by the functions MA(MVA) and MB(MVA), which are Boolean integers. They are obtained from the truth state of MVA — viz. MSTR, MSFL etc by using these functions. Vice versa, if we wish to find the truth state of a vector MVA given its Boolean components (MAA, MBB) we use the subprogram MSTATE(MAA, MBB).

(iii) Matrix operators:

The 16 basic 2×2 matrices are given the general name MZKL where L = E or M according as it is a normal operator, or the complemented operator, and K stands for the one-letter symbol

of the logical operator which it represents. The letter Z following M is used to indicate the fact that it is an operator, just as V following M is used to represent that it is a term (V is the first letter of "vector"). The letter M is used invariably in MATLOG to avoid any possible confusion with the NYAYA operators, or terms, in case a translation from one to the other is required.

Each matrix MZKL obviously has 4 elements — namely the elements $\alpha\alpha$, $\alpha\beta$, $\beta\alpha$, and $\beta\beta$. Instead of representing these in terms of two symbols α and β , they are simply called as the components K1, K2, K3, and K4 of MZKL. The corresponding Boolean elements are obtained using the FORTRAN functions KK1(MZKL), KK2(MZKL), KK3(MZKL), KK4(MZKL). The list of these components K1, K2, K3, K4 and the nature of the matrix corresponding to all the 16 logical operators representable by 2 x 2 matrices are given in Table 2. In the foot note to the table the full names of each operator in terms of the symbols K and L are explained.

3. Matrix Interpretation of Logical Operations

(a) Classical operators

(i) Unary operators:

We know that unary logical relation of the type

$$\underline{\underline{a}} \text{ } Y = \underline{\underline{b}} \quad (16)$$

can be written in the vector-matrix formalism as

$$\langle \underline{a} | \underline{Y} | = \langle \underline{b} | \quad (17)$$

in which $\langle \underline{a} |$ is a two-element Boolean vector and $|\underline{Y}|$ is a 2×2 matrix. The corresponding statement in MATLOG takes the form

$$MVB = MUNN(MVA, MZYB) \quad (18)$$

It will be seen that it is a very close translation of (17) with only the form of the logical operator namely that it is unary normal being specified in the name of the function. Similarly, if we wish to obtain the corresponding transposed relation

$$\langle \underline{b} | \underline{Y} | = \langle \underline{a} | \quad (19a)$$

which is equivalent to

$$\langle \underline{a} | \underline{Y}^t | = \langle \underline{a} | \underline{N} | \underline{Y} | \underline{N} | = \langle \underline{b} | \quad (19b)$$

The corresponding equations can be written in two forms. We

may use the "reverse" operator MZVE of \underline{Y} in (19a), to obtain

$$MVA = MUNN(MVB, MZVE) \quad (20a)$$

Or, we may use the fact that \underline{Y} is the "reverse" or "transpose" of \underline{Y} , so that we use the equation (19b) using \underline{Y}^t , and the transpose of the matrix $|\underline{Y}|$, in the form

$$MVA = MUNT(MVB, MZYE) \quad (20b)$$

When it is written in the form (20b), we mean that the operator is unary, but the transposed form of MZYE. If we look at Table 2, it will be seen that the matrices MZYE and MZVE are transposes of one another, and in the logical sense, they are what we have termed as "reverse" operators of each other, as shown by the relations (17) and (19a) in which one obtains $\langle \underline{b} |$ from $\langle \underline{a} |$ in (17) and $\langle \underline{a} |$ from $\langle \underline{b} |$ in (19a).

In a similar way, when the complement of a matrix is needed, as in Eq. (13b), it is possible to obtain it from the function COMP(MZKL) (see Sec. 4(b)). The above example would indicate the different ways in which a unary relation in logic is converted to the corresponding vector-matrix equation, and written in FORTRAN in MATLOG.

(ii) Binary operators:

Coming now to the case of binary relations, the normal binary relations are treated in the same way as Eqs. (16), (17) and (18). Thus, the connective "and" of classical logic is expressed by the equations

$$\underline{\underline{a}} \wedge \underline{\underline{b}} = \underline{\underline{c}} \quad (21a)$$

The corresponding vector-matrix equation is written in the form

$$\langle \underline{a} | A | \underline{b} \rangle \langle \underline{v} | = \langle \underline{c} | \quad (21b)$$

and this is written in MATLOG in the form

$$MVC = MBDN(MVA, MZAE, MVB) \quad (21c)$$

Again, in the name of the operator, the letter B stands for binary, the letter D for the direct relation and the letter N is used to indicate that the matrix MZAE is used in the normal form as contrasted with the transposed form of it; The mathematics of carrying out the relation (21b) is shown by Eqs. (13a) and (13b) referring to a general operator \underline{A} . Therefore, we shall write here, for clarity, the actual equations for \underline{A} , which are

$$\langle \underline{a} | \underline{A} | \underline{b} \rangle = c_\alpha ; \quad \langle \underline{a} | \underline{A}^c | \underline{b} \rangle = c_\beta \quad (22)$$

The vector-matrix multiplications, and the calculation of the two Boolean Dirac brackets, can be implemented by using the subroutines described in Section 4(b).

The transposed form of the operator (say \underline{A}^t) is required under certain conditions, and we can, using a notation similar to that for the unary operator, write the MATLOG statement

$$MVD = MBDT(MVA, MZAE, MVB) \quad (23a)$$

with N in MBDN replaced by T in MBDT.

This will be equivalent to the logical statement

$$\underline{\underline{a}} \underset{\sim}{\overset{A^t}{\sim}} \underline{\underline{b}} = \underline{\underline{c}} \quad (23b)$$

Considering next, the reverse binary connectives, the logical statement has the typical form (for "reverse and") :

$$\underline{\underline{c}} \overset{\leftarrow}{\underset{\sim}{\sim}} \underline{\underline{a}} = \underline{\underline{b}} \quad (24a)$$

The corresponding MATLOG statement is

$$MVB = MBRN(MVC, MZAE, MVA) \quad (24b)$$

The important point to be noticed is that just as the arrow is put over the symbol \sim to indicate that it is the binary reverse operator, the MATLOG name of the operator has the letter R in MBRN, where B stands for binary, and R stands for reverse, the N of course indicating that the matrix is used as such without transposing it.

The actual working out of the vector $\underline{\underline{b}}$ follows the principles of SNS logic which may be stated in matrix notation as follows :

$$\text{If } \underline{\underline{c}} = \underline{\underline{T}}, \quad \langle \underline{\underline{a}} | \underline{\underline{A}} \rangle = \langle \underline{\underline{b}} | \quad (25a)$$

$$\text{If } \underline{\underline{c}} = \underline{\underline{F}}, \quad \langle \underline{\underline{a}} | \underline{\underline{A}}^C \rangle = \langle \underline{\underline{b}} | \quad (25b)$$

$$\text{If } \underline{\underline{c}} = \underline{\underline{D}}, \quad \underline{\underline{b}} = \underline{\underline{D}} \quad (25c)$$

and

$$\text{If } \underline{\underline{c}} = \underline{\underline{X}}, \quad \underline{\underline{b}} = \underline{\underline{X}} \quad (25d)$$

The implementation of these is described in Section 4, and the full program for this function MBRN is given in the Appendix.

If one has to obtain the value of $\underline{\underline{a}}$, given the truth values of $\underline{\underline{b}}$ and $\underline{\underline{c}}$, given that the relation $\underline{\underline{a}} \underset{\sim}{\sim} \underline{\underline{b}} = \underline{\underline{c}}$, exists, then a procedure very similar to the above is employed, but we have to write the equation for the reverse relation in the form :

$$\underline{\underline{c}} \underset{\sim}{\sim}^t \underline{\underline{b}} = \underline{\underline{a}} \quad (26a)$$

The corresponding MATLOG function giving $\underline{\underline{a}}$ (MVA) has the form

$$\text{MVA} = \text{MBRT}(\text{MVC}, \text{MZA}, \text{MVB}) \quad (26b)$$

where the letter T in MBRT indicates that $\underset{\sim}{\sim}^t$ is to be used.

The great advantage of the four types of binary operators given in (21), (23), (24) and (26) is that they are extremely

useful when one has the need to go from the direct form of the relation to the reverse form, one can then write the equation to give the result of using the output of the direct relations and either of the other two as inputs, as required. The writing down of the program for such processes is greatly facilitated by having these four types of binary operators.

(b) Simple SNS functions

In addition to the above unary and binary operators, the operation of negation either in the form of $\underline{\sim}^N$, or $\underline{\sim}^M$, is frequently encountered, and it would be worthwhile having very simple functions for these. Hence simple MATLOG functions, closely similar to their NYAYA forms, are also available for these two connectives as shown in (27a) and (b) :

$$\underline{\sim}^N = \underline{\equiv} \quad \text{is} \quad \text{MVB} = \text{MON(MVA)} \quad (27a)$$

and

$$\underline{\sim}^M = \underline{\equiv} \quad \text{is} \quad \text{MVB} = \text{MOM(MVA)} \quad (27b)$$

(c) Purely SNS operators

As has been mentioned in [3], classical logic leads to the

need for the postulation of other operators which are particularly relevant only in SNS logic, such as M , U , W and G . These cannot be expressed by 2×2 matrices, but they can be expressed simply by making use of the Boolean addition, multiplication, equation and complementation, of 2-element vectors. Therefore, the form of the functions representing these connectives are very similar to that used in NYAYA. However, for the sake of uniformity, their names and formats are made closely similar to those adopted for the unary and binary classical operators involving all the 16 matrices. Thus, MUSN, will stand for a unary SNS (normal) operator, while MBSN will represent a binary SNS (normal) operator. The vectors that are connected by the relevant operators are put in the matrix form, although the actual logical operations performed on them do not involve matrix multiplication. Thus, two sub-programs are available for the four connectives of SNS logic mentioned above :

$$\text{MVB} = \text{MUSN}(\text{MVA}, \text{MZSM}) \text{ for } \text{M} \quad (28a)$$

$$\text{MVC} = \text{MBSN}(\text{MVA}, \text{MZSW}, \text{MVB}) \text{ for } \underline{W} \quad (28b)$$

$$\text{MVC} = \text{MBSN}(\text{MVA}, \text{MZSU}, \text{MVB}) \text{ for } \underline{U} \quad (28c)$$

$$\text{MVC} = \text{MBSN}(\text{MVA}, \text{MZSG}, \text{MVB}) \text{ for } \underline{G} \quad (28d)$$

For ready reference the algebraic operations that are performed for each of these are given below :

$$\underline{\underline{a}} \underline{\underline{M}} = \underline{\underline{b}} ; \quad \underline{a}_{\alpha}^C = \underline{b}_{\alpha} , \quad \underline{a}_{\beta}^C = \underline{b}_{\beta} \quad (29a)$$

$$\underline{\underline{a}} \underline{\underline{W}} \underline{\underline{b}} = \underline{\underline{c}} ; \quad \underline{a}_{\alpha} \otimes \underline{b}_{\alpha} = \underline{c}_{\alpha} , \quad \underline{a}_{\beta} \otimes \underline{b}_{\beta} = \underline{c}_{\beta} \quad (29b)$$

$$\underline{\underline{a}} \underline{\underline{U}} \underline{\underline{b}} = \underline{\underline{c}} ; \quad \underline{a}_{\alpha} \oplus \underline{b}_{\alpha} = \underline{c}_{\alpha} , \quad \underline{a}_{\beta} \oplus \underline{b}_{\beta} = \underline{c}_{\beta} \quad (29c)$$

$$\underline{\underline{a}} \underline{\underline{G}} \underline{\underline{b}} = \underline{\underline{c}} ; \quad \text{If } \underline{\underline{a}} = \underline{\underline{b}}, \text{ then } \underline{\underline{c}} = \underline{\underline{T}}, \text{ otherwise } \underline{\underline{F}} \quad (29d)$$

4. Brief description of MATLOG subprograms

The functions and sub-programs mentioned in Sections 2 and 3 have been implemented in FORTRAN in our MATLOG program. A brief description of each sub-program, giving only the essential algebraic steps, but omitting the details, are given in this section. (The listing of these is given in the Appendix.) In Section 5, we shall indicate how these are applied to actual problems, and illustrate it with a few examples.

(a) Vector and Matrix Components

The first eight function sub-routines are intended for obtaining the α - and β -components of a vector \underline{a} (MVA), and for obtaining the state of the vector given its components MAA and MBB along with the corresponding functions for the components of a matrix, and for obtaining the matrix given the components.

The first two, namely MA(MVA) and MB(MVA), consist in making MA = 1 for the states MSTR and MSDF, and making MB = 1 for MSFL and MSDE and putting them equal to 0 otherwise. In this way, the four possible vectors (1 0), (0 1), (1 1) and (0 0) are obtained and named. When the state of the vector is to be obtained from the components, we use the function MSTATE(MAA,MBB).

As mentioned in Section 2, the four logical constants are given the names MSTR, MSFL, MSDF, MSXX under which are stored the constants 'T', 'F', 'D', 'X' respectively using the statement :

```
DATA MSTR, MSFL, MSDF, MSXX/ 'T', 'F', 'D', 'X' /
```

These four names are declared as common to all modules under the

name MS using the statement :

```
COMMON / MS/ MSTR, MSFL, MSDF, MSXX
```

Again, as mentioned in Section 2, the matrices are represented by four letter names, in general MZKL. Here we have defined a 16 x 5 matrix of name MATDAT(16,5), whose first column contains the 16 matrix names as a string of constants, and the next four columns contain the components (K1, K2, K3, K4) of the corresponding matrix. The structure of the matrix is given in Table 3. The purpose of giving the matrix names as constants is so that we can input matrix names also, just as we input T, F, D, X for a term. This matrix MATDAT is declared common to the modules in the name MATD. The corresponding DATA and COMMON statements are as follows :

```
DATA MATDAT/ 'MZEE', 'MZEM', 'MZAЕ', 'MZAM', 'MZYM', 'MZYЕ'  
    'MZVM', 'MZVE', 'MZOM', 'MZOЕ', 'MZRE', 'MZRM', 'MZCE'  
    'MZCM', 'MZDE', 'MZDM'  
    1, 0, 1, 0, 0, 1, 0, 1, 0, 1, 1, 0, 1, 0, 1, 0,  
    0, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 1, 1, 0,
```

Table 3 : MATDAT

Col 1	Col 2	Col 3	Col 4	Col 5
'MZEE'	1	0	0	1
'MZEM'	0	1	1	0
'MZAE'	1	0	0	0
'MZAM'	0	1	1	1
'MZYM'	0	1	0	0
'MZYE'	1	0	1	1
'MZVM'	0	0	1	0
'MZVE'	1	1	0	1
'MZOM'	0	0	0	1
'MZOE'	1	1	1	0
'MZRE'	1	1	0	0
'MZRM'	0	0	1	1
'MZCE'	1	0	1	0
'MZCM'	0	1	0	1
'MZDE'	1	1	1	1
'MZDM'	0	0	0	0

0, 1, 0, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 1, 0,
1, 0, 0, 1, 0, 1, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0/

COMMON /MATD/MATDAT

Table 3 - Matdat

To have the matrix names, MZKL, as variables, we define a DATA statement which stores the matrix names as constants 'MZKL' :

```
DATA MZEE, MZEM, MZAE, MZAM, MZYM, MZYE, MZVM, MZVE, MZOM,  
      MZOE, MZRE, MZRM, MZCE, MZCM, MZDE, MZDM/ 'MZEE', 'MZEM',  
      'MZAE', 'MZAM', 'MZYM', 'MZYE', 'MZVM', 'MZVE', 'MZOM',  
      'MZOE', 'MZRE', 'MZRM', 'MZCE', 'MZCM', 'MZDE', 'MZDM'/
```

For the SNS operators M, W, U, G, we have given names as MSMM,
MSWW, MSUU, MSGG using the DATA statement :

```
DATA MSMM, MSWW, MSUU, MSGG/ 'M', 'W', 'U', 'G'/
```

All these DATA statements and COMMON statements are in a separate file LIST.FOR and the subprograms are in MATLOG.FOR.

The four components $Z_{\alpha\alpha}$, $Z_{\alpha\beta}$, $Z_{\beta\alpha}$, $Z_{\beta\beta}$, named respectively as the components KK1, KK2, KK3, KK4 of the matrix MZKL, are readily defined in terms of the matrix data given above. They are contained in Item 4 under functions. Similarly, for getting

the matrix from the components one uses the function
MAT(K1, K2, K3, K4).

(b) Functions and sub-programs for vector-matrix operations

These are illustrated under Items 9 to 20 in the Appendix 1b.
They help to obtain several Boolean operations made on scalars,
vectors, and matrices, conversion of an ordinary integer into a
Boolean number, obtaining the transpose of a matrix, the vector-
matrix product, the matrix-vector product and the matrix-matrix
product.

The integer function BOOLAN(IX) converts any positive integer
into the Boolean value, which can be one of the two possible
values 0 and 1. The idea is that if IX is not zero, then its
Boolean value is 1. In the same way, the complement COMPN(N)
of the scalar Boolean number N is obtained by finding the value
 $(1 - N)$ of the Boolean number N.

Just as the complement of a scalar Boolean number is obtained,
the Boolean operation of complementation can be performed on the

elements of a vector, or a matrix, as desired. The corresponding integer functions are

COMPV(MVA) and COMP(MZKL),

In the former case, each component MA(MVA) and MB(MVA) is converted into its Boolean complement. In the latter case, the four components KK1, KK2, KK3, and KK4 are converted into the complement L1, L2, L3, L4 (with LJ = 1 - KKJ). For obtaining the transpose of a 2 x 2 matrix, no special program is written; but the transposed matrix is defined as

TRAN = MAT(KK1(MZKL), KK3(MZKL), KK2(MZKL), KK4(MZKL))

There is also a need for the transpose of the complement of a matrix which is given the name TRCP(MZKL) and it is simply obtained by applying the two operations of COMP and TRAN one after the other in the form

TRCP = TRAN(COMP(MZKL))

The truth value of a vector, or a logical term, is occasionally

needed and we define it as having the values 1 for T, 0 for F, 1/2 for D and 8 for X. The first three are obvious, while the last "impossible" state is given an impossible truth value which occurs outside the allowed range 0 to 1 for T(MVA). Corresponding to the function T(MVA) we have the inverse integer function VEC(TMVA) which gives the state of the vector in MATLOG notation, given the truth value T(MVA).

We now come to a series of integer functions giving products of two vectors, a vector with a matrix, a matrix with a vector, and a matrix with a matrix, using Boolean multiplications and additions. These are respectively given the names

BOLVVP (MVA, MVB) (No. 17)

BOLVMP (MVA, MZKL) (No. 18)

BOLMVP (MZKL, MVA) (No. 19)

and

BOLMMP (MZXY, MZYY) (No. 20)

The letter BOL stand for "Boolean" and VVP, VMP, etc for vector-vector product, vector-matrix product, etc. The details

of the sub-routines are obvious and require no explanation.

(c) Standard unary and binary connectives in MATLOG

These are six in number, and are given under items 21 to 26.

The contents of each of the sub-routines is very short since they use one, or the other of the vector-matrix multiplication functions defined under numbers 17 to 20. We will therefore merely mention them, and not give any details. In actual practice, in some of the cases, where more than one function of this type has to be called for, it is found more suitable to write the full expressions in the sub-routine itself instead of calling the other functions that are needed. This will become clear on inspection of the programs.

The nature of the four functions MUNN(MVA, MZKL), MUNT(MVA, MZKL), MBDN(MVA, MZKL, MVA), MBDT(MVB, MZKL, MVA), MBRN(MVC, MZKL, MVA), MBRT(MVC, MZKL, MVB) have been mentioned in terms of their logical properties in Section 3. The writing of the lines in the sub-routines closely follows the algebraic

definition of these functions, given in Section 3. They are therefore not described.

However, it should be mentioned that we have at our disposal, using only this small number of six functions, the possibility of working out the whole set of logical relations that can be expressed in terms of classical logic operators which are describable by 2×2 matrices, and also to work out the properties of these relations in reverse. The description of the theory of all these is given in Ref. 3.

(d) Other unary and binary functions for logical connectives

We have also made available shortened forms for the functions representing the logical connectives E, N and M, as contained in Item 27 for MOE(MVA), Item 28 for MON(MVA) and Item No. 29 for MOM(MVA). On the other hand, for the SNS operators (both unary and binary), we use the formal functions MUSN(MVA, MSNN) (No. 30, and MBSN(MVA, MSNN, MVB) (No. 31). For convenience in using these matrix representations for various purposes involving graph

theory (such as for computer display of logical graphs), the generic names of the SNS operators also contain four letters and they also start with M. The second letter is U for unary, and B for binary, with the third letter being S, indicating that it is an SNS operator. The fourth letter N in MUSN and MBSN indicates that they are both "normal" connectives, and not reverse connectives. The individual name of the operator is also given a form similar to that for a matrix (MZKL) in that it has also four letters, (MSNN), the second letter S standing for the SNS nature of the operator and NN for "name". To call any particular operator, MSNN is made equivalent to 'M', 'W', 'U', 'G', as the case may be. The way in which these are facilitated will be seen by examining Items 30 and 31 in the listing.

The great merit that MATLOG has in preference to NYAYA is that there is no need to have a special program written for each logical operator according to its properties. Similarly, we can write the corresponding programs for the reverse operators, the

negated operators and so on, with very little trouble, and in a general way. Thus, they are discussed from a unified point of view by representing them as 2×2 matrices which are utilised in only 3 or 4 standard types — namely unary normal, unary reverse, binary normal and binary reverse — taking into account, of course, also the possibility that a matrix may be required in the transposed form for taking care of reversals under particular circumstance. Thus, $(\underline{\underline{a}} \wedge \underline{\underline{b}})N = \underline{\underline{d}}$ is written in MATLOG as

MVD = MQN(MBDN(MVA, MZAE, MVB))

or = MBDN(MVA, MZAM, MVB)

and $\underline{\underline{c}} \leftarrow \underline{\underline{a}} = \underline{\underline{b}}$ as

MVC = MBRN(MVC, MZOE, MVA)

The additional operators that are required only for SNS logic, will require 4×4 matrices if they are expressed strictly in the MATLOG notation. They are, however, treated in a simple ad hoc manner; however, with the form of the function, and its name in MATLOG, being made very similar to those for the matrix operators. It should be mentioned that, if the full set of 4×4 matrices

are used, then the possible different types of operators and states that will have to be considered will become enormously large. They do not seem to find any application, or use, in the currently used types of logical arguments. However, it may be worthwhile examining the properties of such operators, making use of the facilities of computerized programs, because the equations can be written in a form closely similar to those discussed in this report. This is reserved for a future study.

In the next section, we shall consider some examples of problems where MATLOG is found to be particularly useful.

5. Application of MATLOG to arguments in practical problems in logic.

(a) Three simple problems

In order to check the utility and convenience of MATLOG for solving problems, it was applied to three problems discussed in [2].

- (i) Detective problem — detailed solution
- (ii) Detective problem — shortened procedure
- (iii) Problem taken from Stoll's book.

Table 4a

```
INITIATION MVF(2),MVQ(2),MUR(2)
DATA MVEQ,MVU,MUR//T,F,T,F,T,F/
WRITE (3,8)
8 FORMAT (1X,10X,'TRUTH TABLE FOR THE DETECTIVE')
FORMAT (1X,3X,A1,3X,B1,3X,C1,3X,D1,3X,E1,3X,F1)
DO 5 I=1,2
DO 5 J=1,2
DO 5 K=1,2
MVF = MBPN(MVF(I),MZAE,MVQ(J))
MVQ = MBPN(MVF(I),MZAE,MUR(K))
MUR = MBPN(MVF(I),NZEM,MUR(K))
MVU1 = MBSN(MVA,MSOC,MSTR)
MVU2 = MBSN(MVB,MSGG,MSTR)
MVU3 = MBSN(MVC,MSGG,MSTR)
MVU4 = MBSN(MVU1,MSUU,MVU2)
MVX = MBSN(MVU4,MSUU,MVU3)
WRITE (3,4) MVF(I),MVQ(J),MUR(K),MVA,MVB,MVC,MUX
FORMAT (/21X,3(3X,A1),2X,3(3X,A1),5X,A1)
CONTINUE
STOP
END
```

Table 4b

TRUTH TABLE FROM THE DEDECTIVE PROBLEM

P	Q	R	S	T	C	X
T	T	T	F	F	F	D
T	T	F	T	T	T	T
T	F	T	F	F	T	D
T	F	F	T	T	F	U
F	T	T	T	F	F	D
T	T	F	T	F	T	D
F	F	T	F	F	T	U
F	F	F	F	F	F	F

Table 5a

Table 5b

WIDDER TRUTH TABLE FOR THE DETECTIVE PROBLEM

R	P1	Q	P2	P
F	X	F	T	X
F	T	T	D	T

Table 6a

```
DIMENSION MVP(2),MVI(2),MVC(2)
DATA MVP,MVI,MVC//'T','F','T','F','T','F'//
WRITE(3,41)
FORMAT(20//) BX,'TRUTH TABLE FOR THE PROBLEM',
C TAKEN FROM STOHL'S BOOK//23X,'P',3X,'I',3X,'C',5X,'S',
C 3X,'U',3X,'W')
DO 2 I=1,2
DO 2 J=1,2
DO 2 K=1,2
MVI = MBRN(MUNN(MVI(I),MZYE),MZDE,MVP(I))
MUS = MBRN(MUNN(MVI(J),MZYE),MZDE,MVC(K))
MUU = MBSN(MUNN(MUS,MZYE),MSWW,MON(MBRN(MSTR,MZAE,MON(MVC(
K))))))
WRITE(3,3)MVP(I),MVI(J),MVC(K),MUS,MUU,MUW
FORMAT(120X,3(3X,A1),2X,3(3X,A1))
CONTINUE
STOP
END
```

Table 6b

FOURTH TABLET FOR THE PROBLEM TAKEN FROM STOLL'S BOOK

P	T	C	S	U	M
I	T	T	D	X	D
T	F	F	T	X	D
F	F	T	D	X	X
T	F	F	D	F	X
F	I	T	D	X	D
F	F	F	T	X	D
F	F	T	D	X	F
F	F	F	D	F	F

The details of these problems are not given here, but the MATLOG program for each of them as fed into the computer, and the outputs obtained, are given in Tables 4a and 4b, 5a and 5b and 6a and 6b, respectively. The symbols for the various terms are the same as in the earlier references and the results and the format of the equations will show the convenience of using the MATLOG notation and formalism.

(b) Solution using MATLOG of a 25-node Logical Graph

In order to test the capability and convenience of MATLOG for solving larger problems, an arbitrary logical graph was drawn, containing 25 nodes, with three inputs \underline{a} , \underline{b} , \underline{c} and three outputs \underline{x} , \underline{y} , \underline{z} . It has 4 unary operators, all UN, consisting of two \tilde{Y} 's, one \tilde{M} and one \tilde{V} , and 7 binary operators, four of them being matrix operators, one $\tilde{A}(BD)$, two $\tilde{Q}'s(BD)$, one $\tilde{A}(BR)$ — and three of them being purely SNS operators, two $\tilde{W}'s(BD)$, and one $\tilde{G}(BD)$. The full graph is shown in Fig.1, and the logical equations of the

Fig.1. Logical graph of the 25-node problem.

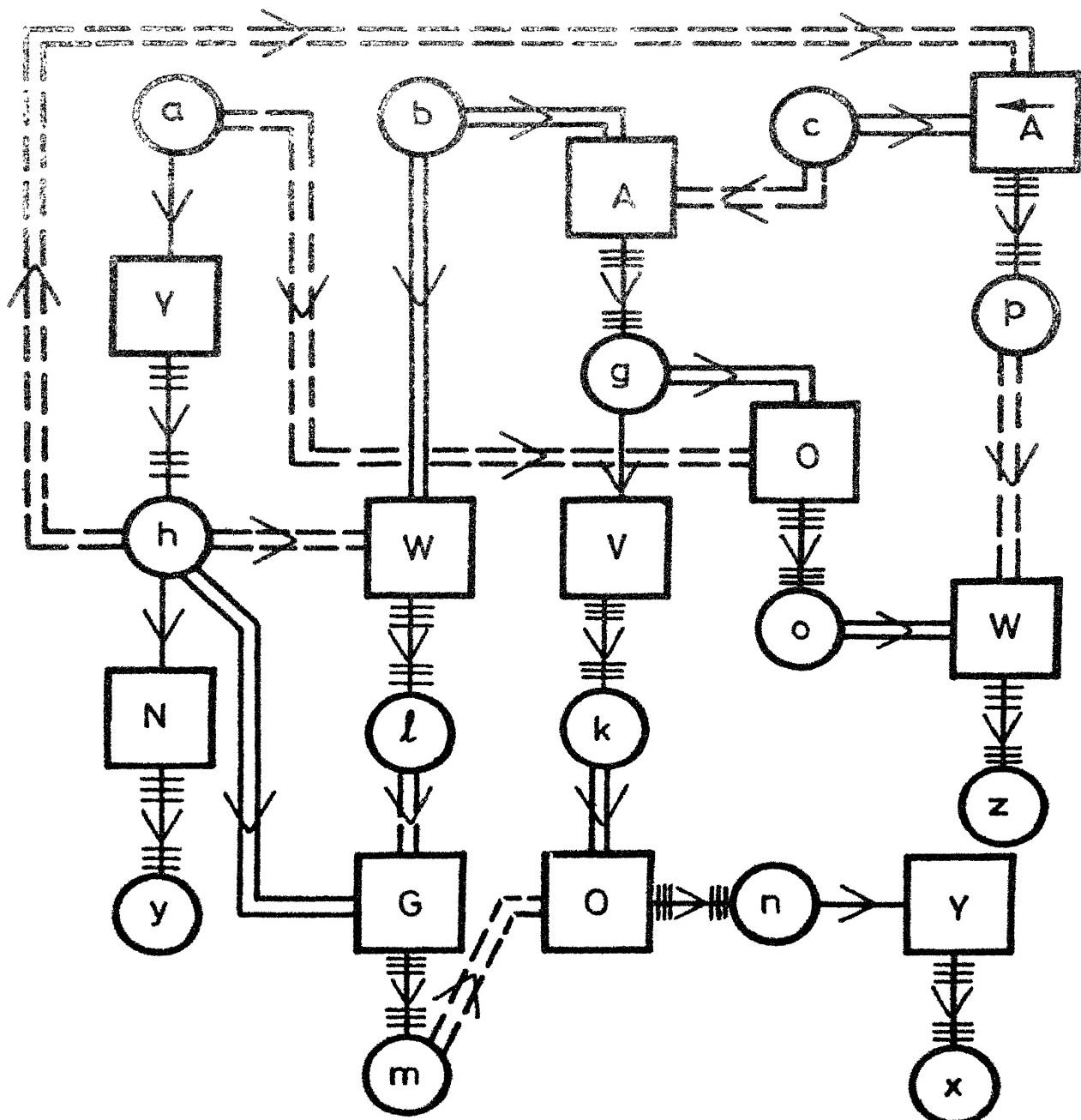


FIG.1. LOGICAL GRAPH OF THE 25-NODE PROBLEM.

argument, written in a sequence in which they can be implemented in MATLOG is shown in Table 7(a). Table 7(b) contains the corres-

Tables 7(a) & 7(b)

ponding FORTRAN statements, and the output from the computer for 27 possible sets of inputs, corresponding to T, F and D for each of the three inputs MVA, MVB, MVC, are listed in Table 8. The

Table 8

time required for the computation on DEC1090 was only 0.03 sec.

It will be noticed that, although three of the seven operators (namely one MZAE, BR; and two MSWW's) can lead to outputs of X states, only 6 of the 27 have at least one output in the impossible state. If only the states T and F are allowed, then 4 of the 8 possible inputs lead to the impossible state for one of the outputs. However, the output y is never X, which is because it is derived from a by means of two unary operations Y and N, which

Table 7(a)

Logical Equations for the 25-node Problem

(Input)	$\underline{\underline{a}} \sim \underline{\underline{y}} = \underline{\underline{h}}$	
(Input)	$\underline{\underline{b}} \sim \underline{\underline{A}} \underline{\underline{c}} = \underline{\underline{g}}$	
	$\underline{\underline{h}} \sim \underline{\underline{N}} = \underline{\underline{y}}$	(Final output)
	$\underline{\underline{g}} \sim \underline{\underline{Q}} \underline{\underline{a}} = \underline{\underline{o}}$	
(Input)	$\underline{\underline{c}} \sim \overset{\leftarrow}{\underline{\underline{A}}} \underline{\underline{h}} = \underline{\underline{p}}$	
	$\underline{\underline{g}} \sim \underline{\underline{V}} = \underline{\underline{k}}$	
	$\underline{\underline{b}} \sim \underline{\underline{W}} \underline{\underline{h}} = \underline{\underline{l}}$	
	$\underline{\underline{o}} \sim \underline{\underline{w}} \underline{\underline{p}} = \underline{\underline{n}}$	(Final output)
	$\underline{\underline{h}} \sim \underline{\underline{G}} \underline{\underline{l}} = \underline{\underline{m}}$	
	$\underline{\underline{k}} \sim \underline{\underline{Q}} \underline{\underline{m}} = \underline{\underline{n}}$	
	$\underline{\underline{n}} \sim \underline{\underline{Y}} = \underline{\underline{x}}$	(Final output)

Table 7b

```

DIMENSION NUA(3),MUB(3),MUC(3)
DATA MUA,MUV,MUL/1.0,1.0,1.0/,F1,'D',T1,'F',F2,'D',T2,'F',F3,'D'/
WRITE (3,2)
2 FORMAT (1H1,1X,15X,'TABLE OF RESULTS FOR THE 25 NODE')
C+PROBLEM/1: 10X,2X,A1,2X,F1,2X,F2,5X,F3,2X,H1,
C,2X,F1,2X,F2,2X,K1,2X,L1,2X,H2,2X,N1,5X,
C,2X,F1,2X,N2,2X,H3/
M1=5,I1=1,J1=3
M2=3,J2=1,K1=3
M3=2,K2=1
MUP=MUN(MUR(J1),MIZAE,MVC(K1))
MUV=MUN(MUW,MIZAE)
MUL=MUN(MUB,MIZAE,MUC(K1))
MVR=MVR(MVC(K1),MIZAE,MVH)
MVC=MBSN(MUD,MZOE,MUP)
MVK=MUN(MVN,MZYAE)
MVB=MBSN(MVB(J1),MSWW,MVH)
MVN=MBSN(MVII,MSGG,MVL)
MVN=MBDN(MVN,MZOE,MVM)
MVX=MUN(MVN,MZYAE)
WRITE (3,4) MUA(I),MUB(J),MUC(K),MUG,MVH,MUD,MUP,MVK,MUL,
CMUM,MUN,MUX,MUV,MVY,MVZ
4 FORMAT (/10X,3(2X,A1),3X,8(2X,A1),3X,3(2X,A1))
CONTINUE
WRITE (3,1000)
1000 FORMAT (10(/))
STOP
END

```

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together cannot give the state $\underline{\underline{X}}$, for all the three states $\underline{\underline{T}}$, $\underline{\underline{F}}$, $\underline{\underline{D}}$ of $\underline{\underline{a}}$.

Thus, we conclude that, if the inputs $\underline{\underline{a}}$, $\underline{\underline{b}}$ and $\underline{\underline{c}}$ are definite, and have the pure states $\underline{\underline{T}}$ or $\underline{\underline{F}}$, then the internal consistency of the argument delineated by this 25-node graph requires that only four possible combinations of these can occur — namely

$$\underline{\underline{T}}, \underline{\underline{T}}, \underline{\underline{T}} ; \quad \underline{\underline{F}}, \underline{\underline{T}}, \underline{\underline{T}} ; \quad \underline{\underline{F}}, \underline{\underline{T}}, \underline{\underline{F}} ; \quad \underline{\underline{F}}, \underline{\underline{F}}, \underline{\underline{F}}$$

If the origin of the contradiction leading to the state $\underline{\underline{X}}$ in the other four cases is examined, and suitable modifications are made, it can be shown that the other four possibilities reduce to one of these. The details of the routine procedure to be followed for doing this is not given in this report as they are still under study. It is hoped that such an analysis, making use of a back-tracing of the graph from the operator, that led to the impossibility, could be made algorithmic, and implemented on the computer by giving appropriate instructions.

However, the general idea may be indicated by taking one example — namely the occurrence of $\underline{\underline{X}}$ for $\underline{\underline{z}}$ in line 2, for the inputs $\underline{\underline{T}}$, $\underline{\underline{T}}$, $\underline{\underline{F}}$. It arises essentially from the contradiction between $\underline{\underline{o}} = \underline{\underline{T}}$ and $\underline{\underline{p}} = \underline{\underline{F}}$, which are the inputs to the $\underline{\underline{W}}$ of node 24, which leads to $\underline{\underline{z}}$ as output. Therefore, we must change either $\underline{\underline{o}}$ to $\underline{\underline{F}}$, or $\underline{\underline{p}}$ to $\underline{\underline{T}}$.

(i) Suppose we make $\underline{\underline{p}} = \underline{\underline{T}}$. Then, since $\underline{\underline{h}} = \underline{\underline{T}}$, the equation $\underline{\underline{c}} \wedge \underline{\underline{h}} = \underline{\underline{p}}$, converted to $\underline{\underline{p}} \wedge \underline{\underline{h}} = \underline{\underline{c}}$, yields $\underline{\underline{c}} = \underline{\underline{T}}$. It is then verified that this change in $\underline{\underline{c}}$ does not produce any change in $\underline{\underline{o}}$, which remains $\underline{\underline{T}}$. Thus, the contradiction is removed, but the input is now $\underline{\underline{T}}$, $\underline{\underline{T}}$, $\underline{\underline{T}}$, which is perfectly satisfactory, as it is free of any contradictions, as seen from line number 1 of Table 8,

(ii) Suppose we make $\underline{\underline{o}} = \underline{\underline{F}}$. Then, the reversal of the equation $\underline{\underline{g}} \wedge \underline{\underline{a}} = \underline{\underline{o}}$, with $\underline{\underline{o}} = \underline{\underline{F}}$, gives the result that $\underline{\underline{a}} = \underline{\underline{F}}$, in addition to $\underline{\underline{g}} = \underline{\underline{F}}$ which is already true. It is readily verified that $\underline{\underline{a}} = \underline{\underline{F}}$ does not produce any other contradiction, for $\underline{\underline{a}} \rightarrow \underline{\underline{h_D}}$ and $\underline{\underline{h_D}} \rightarrow \underline{\underline{p_D}}$, which is a permissible input into

$\stackrel{0}{=} \stackrel{W}{\sim} p = z$ and leads to no contradiction. Thus, in this case, the input becomes F, T, F, which occurs on line number 11 of Table 8, and is free of contradictions, as expected.

The main lines of study that are now being pursued are to examine:-

- (a) How a set of elementary statements (each containing only one unary, or one binary, connective), but not in logical sequence, can be re-arranged in sequence (in an algorithmic procedure) by constructing the logical graph and analyzing it.
- (b) How to make a computer analysis of a contradiction and trace its origin back to its primary source — either to a wrong input statement, or to a discrepancy in some step of the argument itself.

We wish to thank M.V. Manjula and Manjunath for their assistance in preparing this Report.

Appendix

1. (a) Listing of the file LIST.FOR.

C.....PROGRAM LIST.FOR

DIMENSION MATDAT(16,5)

COMMON /MATD/MATDAT

DATA MATDAT/'MZEE', 'MZEM', 'MZAЕ', 'MZAM', 'MZYM', 'MZYЕ',
C'MZVM', 'MZVE', 'MZOM', 'MZOЕ', 'MZRE', 'MZRM', 'MZCE', 'MZCM',
C'MZDE', 'MZDM', 1,0,1,0,0,1,0,1,0,1,1,0,1,0,1,0,0,1,0,1,1,0,
C0,1,0,1,1,0,0,1,1,0,0,1,0,1,1,0,0,1,0,1,1,0,1,0,
C1,0,0,1,0,1,0,1,1,0,0,1,0,1,1,0/

DATA MZEE,MZEM,MZAЕ,MZAM,MZYM,MZYЕ,MZVM,MZVE,MZOM,MZOЕ,
CMZRE,MZRM,MZCE,MZCM,MZDE,MZDM/'MZEE', 'MZEM', 'MZAЕ', 'MZAM',
C'MZYM', 'MZYЕ', 'MZVM', 'MZVE', 'MZOM', 'MZOЕ', 'MZRE', 'MZRM',
C'MZCE', 'MZCM', 'MZDE', 'MZDM' /

DATA MSTR,MSFL,MSDF,MSXX/'T', 'F', 'D', 'X' /

COMMON /MS/MSTR,MSFL,MSDF,MSXX

DATA MSMM,MSWW,MSUU,MSGG/'M', 'W', 'U', 'G' /

1. (b) Listing of MATLOG programs.

PROGRAM MATLOG

I Functions for Vector and matrix components.

1. FUNCTION MA(MVA)
C THIS SUBPROGRAM COMPUTES THE ALPHA COMPONENT OF THE VARIABLE MV.
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
MA = 0
IF ((MVA .EQ. MSTR) .OR. (MVA .EQ. MSDF)) MA = 1
END

2. FUNCTION MB(MVA)
C THIS SUBPROGRAM COMPUTES THE BETA COMPONENT OF THE VARIABLE MVA
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
MB = 0
IF ((MVA .EQ. MSFL) .OR. (MVA .EQ. MSDF)) MB = 1
END

3. FUNCTION MSTATE(MAA,MBB)
C THIS SUBPROGRAM COMPUTES THE MATLOG STATE OF THE VARIABLE MVA
C GIVEN ITS COMPONENTS
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
IF (MAA .EQ. 1) GO TO 1
IF (MBB .EQ. 1) GO TO 2
MSTATE = MSXX;RETURN
2 MSTATE = MSFL;RETURN
1 IF (MBB .EQ. 1) GO TO 3
MSTATE = MSTR;RETURN
3 MSTATE = MSDF
END

4. FUNCTION KK1(MZKL)
C THIS SUBPROGRAM FINDS THE ALPHA-ALPHA COMPONENT OF THE MATRIX

C GIVEN BY THE MATRIX NAME OF MZKL.
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I=1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK1 = MATDAT(I,2);RETURN
2 CONTINUE
END

5. FUNCTION KK2(MZKL)

C THIS SUBPROGRAM FINDS THE ALPHA-BETA COMPONENT OF THE MATRIX
C GIVEN BY THE MATRIX NAME OF MZKL.
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK2 = MATDAT(I,3);RETURN
2 CONTINUE
END

6. FUNCTION KK3(MZKL)

C THIS SUBPROGRAM FINDS THE BETA-ALPHA COMPONENT OF THE MATRIX
C GIVEN BY THE MATRIX NAME OF MZKL.
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK3 = MATDAT(I,4);RETURN
2 CONTINUE
END

7. FUNCTION KK4(MZKL)

C THIS FUNCTION FINDS THE BETA-BETA COMPONENT OF THE MATRIX
C GIVEN BY THE MATRIX NAME MZKL.

```
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK4 = MATDAT(I,5);RETURN
2 CONTINUE
END

8.
FUNCTION MAT(K1,K2,K3,K4)
C THIS SUBPROGRAM COMPUTES THE MATRIX NAME GIVEN ITS ELEMENTS
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (K1 .NE. MATDAT(I,2)) GO TO 2
IF (K2 .NE. MATDAT(I,3)) GO TO 2
IF (K3 .NE. MATDAT(I,4)) GO TO 2
IF (K4 .NE. MATDAT(I,5)) GO TO 2
MAT = MATDAT(I,1);RETURN
2 CONTINUE
END
```

II Functions for Vector-matrix operations.

```
9.
INTEGER FUNCTION BOOLAN(IX)
C THIS SUBPROGRAM FINDS THE BOOLAN EQUIVALENT OF THE INTEGER
C NUMBER IX.
BOOLAN = 1
IF (IX .EQ. 0) BOOLAN = 0
RETURN
END

10.
INTEGER FUNCTION COMPN(N)
C THIS SUBPROGRAM PERFORMS THE COMPLEMENTATION OPERATION
C ON THE NUMBER N
```

```
      COMPN = 1-N
      END

11. INTEGER FUNCTION COMPV(MVA)
C   THIS SUBPROGRAM PERFORMS THE COMPLEMENTATION OPERATION
C   ON THE VARIABLE MVA
      COMMON/MS/MSTR,MSFL,MSDF,MSXX
      COMPV = MSTATE(1-MA(MVA),1-MB(MVA))
      END

12. INTEGER FUNCTION COMP(MZKL)
C   THIS SUBPROGRAM PERFORMS THE COMPLEMENTATION OPERATION ON
C   THE MATRIX MZKL.
      L1 = 1-KK1(MZKL)
      L2 = 1-KK2(MZKL)
      L3 = 1-KK3(MZKL)
      L4 = 1-KK4(MZKL)
      COMP = MAT(L1,L2,L3,L4)
      END

13. INTEGER FUNCTION TRAN(MZKL)
C   THIS SUBPROGRAM PERFORMS THE TRANSPOSE OPERATION ON THE
C   MATRIX MZKL.
      TRAN = MAT(KK1(MZKL),KK3(MZKL),KK2(MZKL),KK4(MZKL))
      END

14. INTEGER FUNCTION TRCP(MZKL)
C   THIS SUBPROGRAM PERFORMS THE TRANSPOSE-COMPLEMENT OPERATION
C   ON MZKL.
      INTEGER TRAN,COMP
      TRCP = TRAN(COMP(MZKL))
      END

15. FUNCTION T(MVA)
C   THIS SUBPROGRAM COMPUTES THE TRUTH VALUE OF THE VECTOR MVA.
```

```
COMMON /MS/MSTR,MSFL,MSDF,MSXX
SQ = MA(MVA)*MA(MVA)+MB(MVA)*MB(MVA)
IF (SQ .EQ. 0.0) GO TO 3
T = (MA(MVA)*MA(MVA))/SQ
RETURN
3 T = 8.0
END

16. INTEGER FUNCTION VEC(TMVA)
C THIS FUNCTION FINDS THE VECTOR MVA, GIVEN ITS TRUTH VALUE TMVA.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
IF (TMVA .EQ. 8.0) GO TO 3
T1 = TMVA; T2 = 1-TMVA
T = (T1*T1+T2*T2)
TA = T1/T; TB = T2/T
VEC = MSTATE ( INT(TA + 0.001),INT(TB + 0.001))
RETURN
3 VEC = MSXX
END

17. INTEGER FUNCTION BOLVVP(MVA,MVB)
C THIS SUBPROGRAM PERFORMS THE BOOLEAN VECTOR-VECTOR PRODUCT
C OF THE VECTORS MVA AND MVB.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
INTEGER BOOLAN
BOLVVP = BOOLAN(MA(MVA)*MA(MVB)+MB(MVA)*MB(MVB))
END

18. INTEGER FUNCTION BOLVMP(MVA,MZKL)
THIS SUBPROGRAM PERFORMS THE OPERATION BOOLEAN VECTOR-MATRIX
PRODUCT OF THE MATRIX MZKL AND THE INPUT VECTOR MVA.
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
INTEGER BOOLAN
MAMVB = BOOLAN(MA(MVA)*KK1(MZKL)+MB(MVA)*KK3(MZKL))
```

```
MBMVB = BOOLAN(MA(MVA)*KK2(MZKL)+MB(MVA)*KK4(MZKL))
```

```
BOLVMP = MSTATE(MAMVB,MBMVB)
```

```
END
```

19.

```
INTEGER FUNCTION BOLMVP(MZKL,MVA)
```

C THIS SUBPROGRAM PERFORMS THE BOOLEAN MATRIX VECTOR PRODUCT
C OF THE MATRIX MZKL ON THE VECTOR MVA.

```
COMMON /MS/MSTR,MSFL,MSDF,MSXX
```

```
INTEGER BOOLAN
```

```
MAMVB = BOOLAN(KK1(MZKL)*MA(MVA) + KK2(MZKL)*MB(MVA))
```

```
MBMVB = BOOLAN(KK3(MZKL)*MA(MVA) + KK4(MZKL)*MB(MVA))
```

```
BOLMVP = MSTATE(MAMVB,MBMVB)
```

```
END
```

20.

```
INTEGER FUNCTION BOLMMP(MZKL,MZKM)
```

C THIS SUBPROGRAM PERFORMS THE BOOLEAN MATRIX-MATRIX
C PRODUCT.

```
INTEGER BOOLAN
```

```
K1 = BOOLAN(KK1(MZKL)*KK1(MZKM)+KK2(MZKL)*KK3(MZKM))
```

```
K2 = BOOLAN(KK1(MZKL)*KK2(MZKM)+KK2(MZKL)*KK4(MZKM))
```

```
K3 = BOOLAN(KK3(MZKL)*KK1(MZKM)+KK4(MZKL)*KK3(MZKM))
```

```
K4 = BOOLAN(KK3(MZKL)*KK2(MZKM)+KK4(MZKL)*KK4(MZKM))
```

```
BOLMMP = MAT(K1,K2,K3,K4)
```

```
END
```

II Standard unary and binary connectives in MATLOG.

21.

```
FUNCTION MUNN(MVA,MZKL)
```

C THIS SUBPROGRAM PERFORMS THE MATRIX UNARY OPERATION MZKL ON MVA.
C THIS IS THE SAME SUBPROGRAM AS BOLVMP.

```
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
```

```
INTEGER BOLVMP
```

```
MUNN = BOLVMP(MVA,MZKL)
```

```
END
```

22.

```
FUNCTION MUNT(MVA,MZKL)
C THIS FUNCTION PERFORMS THE MATRIX UNARY OPERATION OF THE
C TRANPOSE OF THE MATRIX MZKL ON THE INPUT MVA.
```

```
INTEGER BOLVMP,TRAN
```

```
MUNT = BOLVMP(MVA,TRAN(MZKL))
```

```
END
```

23.

```
FUNCTION MBDN(MVA,MZKL,MVB)
C THIS SUBPROGRAM PERFORMS THE BINARY OPERATION CORRESPONDING
C TO THE MATRIX MZKL ON THE INPUT VECTORS MVA AND MVB.
```

```
COMMON /MS/MSTR,MSFL,MSDF,MSXX
```

```
INTEGER COMP,BOOLAN
```

```
MVG1 = MA(MVA)*KK1(MZKL)+MB(MVA)*KK3(MZKL)
```

```
MVG2 = MA(MVA)*KK2(MZKL)+MB(MVA)*KK4(MZKL)
```

```
MAMVC = BOOLAN(MVG1*MA(MVB)+MVG2*MB(MVB))
```

```
MZKL1 = COMP(MZKL)
```

```
MVG1 = MA(MVA)*KK1(MZKL1)+MB(MVA)*KK3(MZKL1)
```

```
MVG2 = MA(MVA)*KK2(MZKL1)+MB(MVA)*KK4(MZKL1)
```

```
MBMVC = BOOLAN(MVG1*MA(MVB)+MVG2*MB(MVB))
```

```
MBDN = MSTATE(MAMVC,MBMVC)
```

```
END
```

24.

```
FUNCTION MBDT(MVB,MZKL,MVA)
```

```
; THIS SUBPROGRAM PERFORMS THE MATRIX BINARY DIRECT OPERATION OF
; THE TRANPOSE OF THE MATRIX MZKL ON THE INPUTS MVB AND MVA.
```

```
COMMON /MS/MSTR,MSFL,MSDF,MSXX
```

```
INTEGER TRAN
```

```
MBDT = MBDN(MVB,TRAN(MZKL),MVA)
```

```
END
```

25.

```
FUNCTION MBRN(MVC,MZKL,MVA)
```

```
THIS SUBPROGRAM PERFORMS THE BINARY REVERSE OPERATION,MZKL
ON MVC AND MVA.
```

```
COMMON /MS/MSTR,MSFL,MSDF,MSXX
INTEGER COMP,BOLVMP
IF (MVA .EQ. MSXX) GO TO 1
IF ((MVC .EQ. MSDF) .OR. (MVC .EQ. MSXX)) GO TO 2
MZRKL = MZKL
IF (MVC .EQ. MSFL) MZRKL = COMP(MZKL)
MBRN = BOLVMP(MVA,MZRKL);RETURN
2 MBRN = MVC;RETURN
1 MBRN = MSXX
END
```

26.

```
FUNCTION MBRT(MVC,MZKL,MVB)
C THIS SUBPROGRAM PERFORMS THE MATRIX BINARY REVERSE OPERATION
C OF THE TRANPOSE OF THE MATRIX MZKL ON INPUTS MVC AND MVB.
COMMON /MS/MSTR,MSF,MSDF,MSXX
INTEGER TRAN
MBRT = MBRN(MVC,TRAN(MZKL),MVB)
END
```

IV Other unary and binary functions for logical connectives.

27.

```
FUNCTION MOE(MVA)
C THIS SUBPROGRAM PERFORMS THE OPERATION EQUAL TO ON THE VECTOR
C REPRESENTED BY MVA.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
MOE = MVA
END
```

28.

```
FUNCTION MON(MVA)
C THIS SUBPROGRAM PERFORMS THE OPERATION NEGATION ON THE
C VARIABLE MVA.
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
MON = MSTATE(MB(MVA),MA(MVA))
END
```

29. FUNCTION MOM(MVA)
C THIS SUBPROGRAM PERFORMS THE OPERATION COMPLEMENTATION
COMMON /MS/MSTR,MSFL,MSDF,MSXX
MOM = MSTATE(1-MA(MVA),1-MB(MVA))
END

30. FUNCTION MUSN(MVA,MSNN)
C THIS SUBPROGRAM PERFORMS THE SNS UNARY OPERATION MSNN ON
C THE INPUT MVA.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
IF (MSNN .EQ. 'M') GO TO 1
RETURN
1 MUSN = MSTATE(1-MA(MVA),1-MB(MVA))
RETURN
END

31. FUNCTION MBSN(MVA,MSNN,MVB)
C THIS SUBPROGRAM PERFORMS THE SNS BINARY OPERATION MSNN
C (K MAY BE W,U,G) ON THE INPUTS MVA AND MVB.
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
INTEGER BOOLAN
IF ((MVA .EQ. MSXX) .OR. (MVB .EQ. MSXX)) GO TO 11
IF (MSNN .EQ. 'W') GO TO 1
IF (MSNN .EQ. 'U') GO TO 2
IF (MSNN .EQ. 'G') GO TO 3
1 MAMVC = MA(MVA)*MA(MVB)
MBMVC = MB(MVA)*MB(MVB)
MBSN = MSTATE(MAMVC,MBMVC)
RETURN
2 MAMVC = BOOLAN(MA(MVA)+MA(MVB))
MBMVC = BOOLAN(MB(MVA)+MB(MVB))
MBSN = MSTATE (MAMVC,MBMVC)
RETURN

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```
3 MBSN = MSFL
IF (MVA .EQ. MVB) MBSN = MSTR
RETURN
11 MBSN = MSXX
END
```

I N F I N I T E N U M B E R O F O S C I L L A T I O N S
I N F O U R I E R T R A N S F O R M S O F
P H Y S I C A L F U N C T I O N S

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INFINITE NUMBER OF CONVERGENCE

IN FOURIER TRANSFORMS OF
PHYSICAL FUNCTIONS

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PREFACE

This is the second report of our studies on Fourier transforms, looked at from physical considerations. The first was MATPHIL Reports No.14, in which the idea of infinite differentiability (ID) of the F.T. ($F(X)$) was shown to be the consequence of the existence of a bounded support (BS) for the function ($f(x)$), which is absolutely integrable (AI). In the same way, this Report No.19 discusses the property of the infinitely oscillatory (IO) nature of the F.T. of a function $f(x)$, which has BS and is AI. It is shown, that, under the same conditions (BS and AI) occurring for $f(x)$, the Fourier transform $F(X)$ is both ID and IO. The consequence is that, if the diffraction pattern of a finite object is cut off beyond an upper limit $|X| = X_1$, and it is reconstructed from this truncated F.T., then the reconstruction always has an infinite number of ripples.

The proof was arrived at in stages, and this Report also grew step by step, as each part of it was prepared from the intermediate theorems that were proved. Although the complete proof has been

obtained and presented in Section 7, it has not been thought worthwhile to rewrite the full presentation since the steps themselves are also interesting from a physical point of view, and will be found useful in particular applications.

There may be a certain amount of repetition in the Report; but we hope that this defect will be excused. A short over-all summary of the main results obtained is given at the end, in Section 8, so that the essential conditions under which the main theorem mentioned above is valid, are brought to the foreground.

After this report was completed, a much simpler and more straightforward proof has been worked out for the case of an analytic $f(x)$ having BS (independent of whether it is ID or not). So, we need consider only two cases: (a) When $f(x)$ or $f(j)(x)$ has two δ -function singularities; (b) when no δ -functions occur and $f(x)$ is analytic in the interval from $-a$ to $+a$. In the latter case, the period of the oscillations, for large X , is $X = 1/2a$, independent of the form of the function $f(x)$.

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1. Introduction

In a previous paper [1], we had shown that if an absolutely integrable (AI) function $f(x)$ is of bounded support (BS), then the Fourier transform $F(X)$ of the function is infinitely differentiable. In fact, $F(X)$ has unbounded support from $X = -\infty$ to $X = +\infty$ and it is also infinitely differentiable at all points X . This necessitates that $F(X)$ is also of bounded variation (BV).

As a simple example, we may consider the rectangular function,

$$f(x) = 1 \text{ for } -a \leq x \leq a \quad \text{and} \quad = 0 \text{ for } |x| > a \quad (1)$$

whose Fourier transform, given by the sinc function

$$F(X) = (\sin 2\pi ax)/\pi X \quad (2)$$

has an infinite number of minima at $X = m/a$, with maxima in between, for the modulus $|F(X)|$

where m an integer. It therefore occurred to us that the existence of an infinite number of oscillations (IO), exhibited by the function in Eq.(2), might be a property of the Fourier transform of any function which is both BS and AI. Such a function $f(x)$ may be called a "physical function", since it can represent the distribution of a physical property (such as mass, or charge density)

over the length of a body of finite size.* (The extension of this to two and three dimensions is obvious, and will not be discussed in this report). It is a common experience that any object of finite size and magnitude exhibits a diffraction pattern which has a series of ripples. Of course, the amplitude of the ripples usually becomes smaller and smaller as $|X|$ increases; but there does not seem to be any mathematical theorem which tells us whether the oscillatory nature of $|F(X)|$ disappears after a certain stage and $|F(X)|$ becomes monotonic for $|X| > X_1$, or whether the ripples continue to occur without any stop upto $|X| = \infty$. We set this question to ourselves and we have proved that the oscillations are infinite in number, right from $X = -\infty$ to $+\infty$, as shown in the following sections.

We shall make a change in notation from that adopted in Matphil Reports No.14. The function (in real space) is denoted by $f(x)$ as before. On the other hand, the Fourier transform of $f(x)$ (in reciprocal space) is denoted by $F(X)$ (as is usually defined in crystallography — see Refs. [2, 3, 4]). When more

* The δ -function $\delta(x-x_0)$ satisfies these properties, since $\int_{-\infty}^{+\infty} \delta(x-x_0)dx$ is finite, and it is non-zero only for $x=x_0$, where x_0 is within the BS.

than one function has to be referred to, we shall use the same letter for a function and its Fourier transform, lower case being used for the function and capitals for the Fourier transform. Thus,

Fourier transform of $g(x)$ is $G(X)$.

Fourier transform of $h(x) = f(x) * g(x)$ is $H(X) = F(X)$ etc.

2. Infinite differentiability of a function at all points.

(a) Relation between change of scale and infinite differentiability (ID)

Since the idea of "infinite differentiability" has been put forward only recently by us [1, 5], we shall give the definition of it here. A function $f(x)$ is said to be infinitely differentiable if it has derivates of all orders, and there exist positive constants K and C such that

$$|f^{(j)}(x)| \leq K C^j, \text{ for all } x \text{ and } j = 1, 2, \dots \quad (3)$$

Under these conditions, the scale used for measuring x can be

redefined, so that

$$x = x/k, \text{ or } x = kx \quad (4)$$

As a consequence, the same functions $f(x)$, and all its derivates $f^{(j)}(x)$ become as follows, when expressed in terms of x' :

$$f(x) = f(kx') = f'(x') \quad (5a)$$

$$\frac{df'(x')}{dx'} = \frac{df(kx')}{dx'} = K \frac{df(kx')}{dx} = k \frac{df(x)}{dx} \quad (5b)$$

Similarly,

$$\frac{d^j f'(x')}{dx'^j} = k^j f^{(j)}(x), \text{ for all } j \quad (5c)$$

Hence, if kC is made < 1 , which can be done since C is finite, then

$$\lim_{j \rightarrow \infty} f^{(j)}(x') \rightarrow 0 \quad (5d)$$

Thus, by a rescaling of x , $f^{(j)}(x)$ can be made into a decreasing function of j for sufficiently large j , and tend to 0 as

$$j \rightarrow \infty$$

The idea of infinite differentiability, as defined by (3), is thus reduced to one in which the magnitude of the j th differential coefficient tends to zero as j increased indefinitely, It also follows that, if a function $f(x)$ is NID, and (3) is not satisfied, then by no change of scale can $f^{(j)}(x)$ be made finite as $j \rightarrow \infty$.

(b) ID more specialized than analyticity

The condition for infinite differentiability may be compared with that for $f(x)$ being analytic, i.e., for $f^{(j)}(x)$ to be finite for all finite j , however large, It is not clearly recognised that analyticity does not demand that $\lim f^{(j)}(x)$ exists for $j \rightarrow \infty$. Even the so-called entire analytic functions which are analytic over the complete complex plane, except at the "point of infinity", do not demand that $f^{(j)}(x)$ is an entire function for $j \rightarrow \infty$. e.g. $f(x) = e^{-x^2}$ is an entire function, but it is not infinitely differentiable.

In fact, as shown in [5], all infinitely differentiable (ID)

functions, which are also absolutely integrable (AI), are also entire functions of the exponential type, which can be defined by

$$|f(z)| \leq K e^{C|z|} \quad (6)$$

However, it should be emphasised that the value of our investigations on functions which are ID does not reside in this reason. In fact, the justification and purpose of studying the property of infinite differentiability and its consequent effects on the other properties of the function $f(x)$, and its Fourier transform $F(X)$, come from the "scale invariance" condition, shown by the transformations between x and x' in Eq. (4). They are fundamental for physics, and the properties of a function and its derivatives cannot depend on the choice of the scale constant k , (or the magnitude of the unit used to measure x). As a consequence, there is the following fundamental difference between ID and NID functions:

For the former

$$\text{ID: } f^{(j)}(x) \rightarrow 0 \text{ as } j \rightarrow \infty \text{ for some } k, \quad (6a)$$

while for the latter

$$\text{NID: } f^{(j)}(x) \rightarrow \infty \text{ as } j \rightarrow \infty \text{ for all } k. \quad (6b)$$

Put in brief logical form,

$$\text{ID : } \exists k \ \exists \lim_{j \rightarrow \infty} f^{(j)}(x) = 0 \quad [\text{Statement A}] \quad (7a)$$

$$\text{NID: } \forall k \ \lim_{j \rightarrow \infty} f^{(j)}(x) \rightarrow \infty \quad [\text{Statement } \neg A] \quad (7b)$$

The two statements are the negations of each other, and,

equivalently, $f^{(j)}(x) \leq K C^j$ for some finite C , in (7a) and
 $f^{(j)}(x) > K C^j$ for all C however large, in (7b).

As mentioned in (4), the former condition can be satisfied for all x , for some chosen K and C . Consequently, we find that

"An ID function is uniformly ID"

and

"A NID function is also NID for all x ".

Consequently, if we denote by \mathcal{C}^j the class of all functions which possess derivatives of all orders, upto and including j , then

$$\text{ID} \iff \mathcal{C}^\infty \quad (7c)$$

and

$$\text{NID} \iff \neg \mathcal{C}^\infty (= \mathcal{C}^0 \cup \mathcal{C}^1 \cup \dots \cup \mathcal{C}^j \cup \dots) \quad (7d)$$

where the ζ_j 's in 7(d) exclude ζ^0 . Thus, among functions that are AI, the class of NTD functions includes all non analytic functions, and also all analytic functions which are not entire functions of the exponential type.

As we shall show in this report, the ID functions, which are necessarily bounded in magnitude and whose FT is a function of bounded support, and hence not analytic, also have the property that they have unbounded support and are infinitely oscillatory (unless they are zero everywhere). The former (UBS) is obvious since they are analytic, while the latter (IO) is extremely interesting and has important physical consequences. Some of these are discussed in the last section 8.

(c) Conditions of absolute integrability (AI) and bounded support (BS)

There is also another restrictive condition which is important in connection with these studies of Fourier transforms, namely the absolute integrability of function say $f(x)$ — i.e, it belongs to the class L^1 . When this happens, it follows

that its Fourier transform $F(X)$ is continuous and always bounded, or

$$|F(X)| \leq L, \text{ a finite number} \quad (8a)$$

and further it is known from standard FT theory that

$$|F(X)| \rightarrow 0, \text{ as } X \rightarrow \pm\infty \quad (8b)$$

Proofs of these may be found in [6, 7]. However, (8b) is true only if $f(x)$ is not a sum of δ -functions (see below). But it does not necessarily follow, from this condition of absolute integrability, that $|f(x)|$ itself is bounded in magnitude, although the Fourier transform $|F(X)|$ is necessarily so. In fact, $f(x)$ can be infinite at certain points x_j provided it is absolutely integrable over a range $x_j - \epsilon$ to $x_j + \epsilon$, ($x_j \neq \pm\infty$) A special example of this situation is found in $\delta(x-x_0)$, which has an integral equal to 1, although its value at the point $x=x_0$ may be unbounded. However, we shall show in Section 4 that the F.T. ($H(X)$) of a sum of δ -functions, $h(x) = \sum c_i \delta(x-x_i)$, does not satisfy the result (8b).

In what has been said above in Sec.2, we have considered

functions $f(x)$ which are infinitely differentiable, and also those that are absolutely integrable. In what follows, we shall assume only the latter property for the function $f(x)$ in real space and consider the nature of its diffraction pattern, or Fourier transform, in reciprocal space. In addition, we also restrict ourselves to functions $f(x)$ of bounded support (BS) (or the type shown in Eq.(1)), defined more generally, as in Eq.(8c) below:

$$\text{B.S. : } f(x) = 0, \text{ for } -\infty < x < -a \text{ and } +a < x < +\infty \quad (8c)$$

In this definition, we may take the support of $f(x)$ to lie from $-a$ to $+a$ without loss of generality, since the origin can be taken anywhere without violating any of the conditions mentioned above.

In Reports 14 and 15, it has been shown that the two properties mentioned above — namely absolute integrability and bounded support of $f(x)$ --- necessarily demand similarly two properties of its Fourier transforms $F(X)$:

- (i) $F(X)$ must have unbounded support, i.e., it does not vanish identically for $|X|$ greater than some finite $|X_1|$.
- (ii) $F(X)$ is infinitely differentiable -- that is to say, all its derivatives should exist and should conform to the condition
- (4) namely $|F^{(j)}(X)| \leq K C^j$ for all j .

3. Infinite number of oscillations of ID functions.

Now, we mention the third condition, which will be proved in this report --- namely THEOREM 1:

If a function $f(x)$, which is absolutely integrable, has bounded support, then its F.T., viz. $F(X)$, in addition to being ID, has an infinite number of oscillations (IO) in its modulus $|F(X)|$ *.

This means that the magnitude of $F(X)$ will increase and decrease an infinite number of times within the range of X which, as we know, is from $-\infty$ to $+\infty$, for the FT of a function of BS & AI. The fact that $F(X)$ is ID under these conditions has already been proved [1, 5]. The result about 10 will be given for a series of special cases of $f(x)$ and then generalised under the most general condition possible, obeying the two restrictions mentioned

* It is likely that $|F(X)|$ is not analytic in some cases, but $|F(X)|^2 = F(X)$ will be analytic, and "IO of $|F(X)|$ " and "IO of $|F(X)|^2$ " will be used, as required, as being interchangeable statements, standing for " $F(X)$ is IO".

in Theorem 1 for $f(x)$ --- namely absolute integrability and bounded support. The special cases which we shall examine may be classified as follows:

a) $f(x)$ consists of a finite number of δ -functions of finite weight. Since the functions $c_i \delta(x-x_i)$ ($i = 1$ to n) have n finite, the coordinates x_i themselves will have necessarily a bounded support. Also the integral of $f(x)$ will be equal to or less than the sum $\sum_{i=1}^n |c_i|$ which will also be finite, since all c_i are finite and their number is finite. Thus, both the conditions required of $f(x)$ are satisfied. In this case, we shall show that the $|F(X)|$ is infinitely oscillatory with undying root-mean-square amplitudes, provided at least two δ -functions with strengths c_1 and c_2 exist. We show this in Section 4.

b) $f(x)$ is analytic between $-a$ and $+a$. This general condition does not seem to be sufficient for our discussion, because of certain restrictions imposed by our method of proof. However, if the function $f(x)$ is even and is infinitely differentiable between $-a$ and $+a$, then $|F(X)|$ can be proved to have an infinite number of oscillations. This is shown in Sec.6.

c) For a general $f(x)$ which is not necessarily symmetric about $x = 0$, we shall adopt a different procedure. Firstly, suppose $f(x)$ is continuous for the whole interval from $-a$ to $+a$ but that it has a finite number of δ -functions at x_i ($i = 1$ to n). Then we can write $f(x)$ in the form

$$f(x) = g(x) + h(x) \quad (9a)$$

where $g(x)$ is continuous between $-a$ and $+a$ and

$$h(x) = \sum c_i \delta(x - x_i) \quad (9b)$$

Then, it follows that

$$G(X) \text{ varies as } 1/X^l \text{ as } X \rightarrow \infty, l \geq 1 \quad (10a)$$

while, by the example in (a),

$$H(X) \text{ has oscillations of finite magnitude as } X \rightarrow \infty \quad (10b)$$

Hence, the Fourier transform $F(X)$ of $f(x)$ in Eq. (9a) has an infinite number of oscillations.

d) We can extend this to the case of discontinuous functions. Then, if no δ -function singularities exist, the discontinuities of $f(x)$ consist of finite jumps d_i at x_i , which correspond to δ -functions $d_i \delta(x-x_i)$ for the first derivative $f^{(1)}(x)$. Now, write $f^{(1)}(x)$ in a form similar to (9a), namely

$$f^{(1)}(x) = g^{(1)}(x) + h^{(1)}(x) \quad (11a)$$

where $g^{(1)}(x)$ consists of a sum of a pieces of continuous functions between x_i and x_{i+1} ; and

$$h^{(1)}(x) = \sum d_i \delta(x-x_i) \quad (11b)$$

by the same conditions as those used for (9a) and (9b) which give (10a) and (10b) it follows that Fourier transform of $f^{(1)}(x)$ in (11a) also has infinite oscillations of finite mag-

nitude as $X \rightarrow \infty$. Now, the F.T. of $f^{(1)}(x)$ is

$$F_1(X) = -2\pi i X F(X) \quad (12a)$$

so that

$$F(X) = -F_1(X)/2\pi i X \quad (12b)$$

also has an infinite number of oscillations, but not of undying amplitude.

e). This can be extended to functions where all derivatives upto order $(j-1)$ have no δ -functions, but $f^{(j)}(x) = g^{(j)}(x) + h^{(j)}(x)$, where $g^{(j)}(x)$ is piecewise continuous, while $H^{(j)}(x)$ is a sum of ξ -functions of the type discussed above. Consequently, we obtain THEOREM 2

"If any derivative $f^{(j)}(x)$ of $f(x)$ contains at least two δ -functions singularities, then it necessarily follows that $F(X)$ has an infinite number of oscillations".

f) We therefore come to the case of functions that have derivatives of all orders, i.e., those functions that are analytic between $-a$ and $+a$. However, if the function is infinitely

differentiable (ID) within this range, even if it is neither symmetric, nor antisymmetric, about $x = 0$, we can generalise the case of even functions discussed in (b) and show that its F.T. has an infinite number of oscillations. This case is discussed in Sec.6(b)(iii) and (iv).

g) Finally, there is the case of analytic functions which have no discontinuity at either $x = -a$ or $+a$, for $f(x)$ and all $f^{(j)}(x)$, but are yet not infinitely differentiable. In that case, clearly

$$f(x) = f^{(1)}(x) = f^{(2)}(x) = \dots = f^{(j)}(x) = \dots = 0, \\ \text{for all } j, \text{ at } x = \pm a \quad (13a)$$

This is the well-known condition for an analytic function to be identically zero everywhere. However, these are all true at $x = \pm a$ for the following function (which, however, does not vanish identically):

$$f(x) = f_1(x) = e^{-1/(a^2-x^2)} \text{ for } -a \leq x \leq a \quad (13b)$$

$$f(x) = f_2(x) = 0, \text{ for } -\infty \leq x \leq -a \text{ & } +a \leq x \leq \infty \quad (13c)$$

The validity of (13a) in this case arises because, at $x = +a$, the left derivatives are all zero for $f_1(x)$, while the right derivatives are all zero for $f_2(x)$, and similarly for $x = -a$. For $f_1(x)$, all $f_1^{(j)}(x) \rightarrow \infty$ for $x - a_+$, so that it is not necessary for $f_1(x)$ to be identically equal to zero everywhere, in spite of (13a) being true for the left limit $x = a_-$. Consequently a special approach has to be tried for functions of this type (See Sec.7).

4. Fourier transforms of a finite number of δ -functions

occurring within a finite range of x

As already mentioned, a function $f(x)$, of BS, will have for its Fourier transform, a function $F(X)$ which is ID and of JBS --- i.e., $F(X)$ exists from $-\infty$ to $+\infty$ of X .

We shall now prove that this function $F(X)$ also has an infinite number of maxima and minima in its modulus. We shall do this in a semi-intuitive way in this paper.

We start with a set of $n \delta$ -functions of weight w_j at x_j , whose F.T. is :

$$F(X) = \sum_1^n w_j e^{2\pi i x_j X}, \quad w_j \text{ real}, \quad x_j \text{ real} \quad (14)$$

Then it follows that

$$|F(X)|^2 = \sum_1^n w_j^2 + \sum_{i=1}^n \sum_{j=1}^n w_i w_j \cos 2\pi(x_i - x_j)X \quad (15a)$$

$$= \sum_{i=1}^n w_j^2 + \sum_{k=1}^m c_k \cos 2\pi y_k X, \quad m = \frac{n(n-1)}{2} \quad (15b)$$

where $c_k = \sum_{i \neq j} w_i w_j$, $y_k = (x_i - x_j)$, all y_k can be taken to be +ve $(15c)$

Since $\sum w_j^2$ is a constant, say C , the variable part of $|F(X)|^2$ can arise only from the second term of (15b). We shall therefore examine this and call this function as

$$H(X) = \sum_{k=1}^m c_k \cos 2\pi y_k X \quad (16)$$

It is obvious that each cosine function will vary from +1 to -1, and back again to +1, in cycles. The wavelength of the cycles, say $L_k (= 1/y_k$ in reciprocal units), are all finite, since we have assumed that the δ -functions are all separate, so that there will be a minimum non-zero value for $y_k = (x_j - x_j)$.

Consequently, the largest wavelength $L_k(\max)$ is finite, and if we take a length L larger than a sufficiently large multiple of this, it follows that the mean value of $H(X)$ ($\langle H(X) \rangle$) is nearly zero, by (17):

$$H(X) = \frac{1}{L} \left\{ \int_{X_1}^{X_1+L} H(X) dX \right\} \approx 0, \text{ for all } X_1 \quad (17)$$

We are not interested in the exact magnitude of L but if we let L to tend to ∞ , it is clear that the mean value of $H(X)$, as defined by (17), will be exactly 0, or as close to it as desired. Note also, that, from (15b), the mean value of $|F(X)|^2$ is

$$\langle |F(X)|^2 \rangle = \sum_{j=1}^n w_j^2 = c \quad (18)$$

For simplicity, denote $|F(X)|^2$ by $I(X)$ (intensity, as it is known in optics and crystallography). We then wish to find the mean square value of the fluctuations of $I(X)$ about its mean value c . Denote $(I(X) - \langle I(X) \rangle)$ by $\Delta I(X)$, which is given by $H(X)$ of (16). Hence the mean square fluctuation of intensity is $\langle H^2(X) \rangle$. Now, from (16),

$$H^2(X) = \sum_{k=1}^m \sum_{l=1}^m c_k c_l \cos 2\pi y_k X \cos 2\pi y_l X \quad (19a)$$

Here again, c_k are finite positive quantities and the mean value of the product of the two cosines occurring in Eq. (19a) taken over a suitable finite range X_1 to X_1+L , can again be made as small as we like, so long as $k \neq l$. Therefore the only contribution to the mean of $H^2(X)$, ($\langle H^2(X) \rangle$), comes from the following:

$$\begin{aligned} \langle H^2(X) \rangle &= \sum_{k=1}^m c_k^2 \cos^2 2\pi y_k X \\ &= \frac{1}{2} \sum_{k=1}^m c_k^2 + \frac{1}{2} \sum_{k=1}^m c_k^2 \cos 4\pi y_k X \end{aligned} \quad (19b)$$

Once again, we see that the first term on the r.h.s. of (19b) is a constant, which we shall indicate by S^2 , while the second, which is a sum of cosines, will all average to zero if L is made large enough. Hence, under the same conditions within which we found that

$$\langle H(X) \rangle = 0 \quad (20a)$$

we also have that

$$\langle H^2(X) \rangle = S^2 \quad (\text{non-zero}) \quad (20b)$$

We shall now discuss the consequences of these two results (20a) and (20b). Taking the former, namely that the mean of $H(X)$ is zero, it means that the function $H(X)$ must be as often positive as negative. If it oscillates between +ve and -ve values somewhere beyond X_1 , then it is clear that $H^2(X)$ will oscillate between 0 and some positive value, and S^2 will be non-zero. On the other hand, if $H(X)$ does not oscillate, then the only way its mean value can be zero is by the function itself vanishing throughout beyond a certain X_1 . But, in this case, the mean value of $H^2(X)$ ($=S^2$) will also be zero, which disagrees with (20b), namely that S^2 is non-zero. The only way this contradiction can be avoided is by all c_k^2 becoming zero as in (20c) below:

$$H^2(X) = S^2 = \frac{1}{2} \sum_{k=1}^n c_k^2 = 0 \quad (20c)$$

But, by (15c), $c_k = 2w_i w_j$ where i and j range over 1 to n , with however i being not equal to j . Hence, either $w_i = 0$ or $w_j = 0$, for each pair $i \neq j$. Thus at most one of the δ -functions can have non-zero weight, if $|F(X)|$ does not have oscillations beyond

x_1 for all values of X .

Also, it follows that, if two, or more, of them have non-zero weight, then there is at least one oscillation for $|X| > |x_1|$, for all X_1 . Also, the root mean-square amplitude of the oscillations about $c = \sum_1^m c_j^2$, will be of the same magnitude S over any range, L of X sufficiently large (from x_1 to x_1+L), so that the oscillations do not die away as X increase, but are of undying (root mean square) amplitude.

This is the result which is vital to the succeeding sections. If $f(x)$ is the sum of two, or more, δ -functions, then its FT (namely $F(X)$) will have undying oscillations of r.m.s. amplitude S , given by

$$S = \left[\sum_{l=1}^n \sum_{j=1}^n w_i^2 w_j^2 \right]^{\frac{1}{2}} \quad (21)$$

$i \neq j$

The above discussion which was restricted to $F(X)$, as defined in (14) with w_j real, is readily extendable to the case where w_j are either complex or real. One has only to write the complex w_j

$$w_j = |w_j| e^{i\alpha_j} \quad (22)$$

where, following crystallographic practice, we shall call α_j as the phase of the wave, with weight $|w_j|$. Then the cosine terms in (15a) take the form

$$\cos [2\pi(x_i - x_j)x + (\alpha_i - \alpha_j)] \quad (23a)$$

$$= \cos (2\pi y_k x + \beta_k) \quad (23b)$$

$$\text{with } \beta_k = (\alpha_i - \alpha_j) \quad (23c)$$

A very simple manipulation of the expression (15b), using this enables us to obtain the result

$$|F(x)|^2 = \sum |w_j|^2 + 2 \sum_{k=1}^m c_k \cos \beta_k \cos 2\pi y_k x \quad (24)$$

Since the quantities $(c_k \cos \beta_k)$ are again a set of constants which may be labelled as c'_k , all the discussion that has been made above for the case when w_k are real, is equally valid for the case where w_j are complex, but $\sum_1^n |w_j|^2$ is finite.

Note: The F.T. of a single δ -function at x_0 is $F(x) = ae^{i2\pi Xx_0}$ and its modulus $|F(x)|$ is a constant (a) for all X from

$-\infty$ to $+\infty$. Although it has no maxima or minima, for our discussion it is considered to be an ID function, since $dF(X)/dX = 0$ at all points (i.e. at an infinity of points). This singular case of an F.T. of constant modulus will be treated as being ID for all purposes in this report.

5. Extension to general functions of bounded support, not ID

(a) Continuous functions (with δ -functions)

We now consider continuous functions existing from $-a$ to $+a$, which may have, in addition, a finite number of δ -function singularities of the type considered in the last section. Then, $f(x)$ is of the form

$$f(x) = g(x) + h(x) \quad (26a)$$

where $g(x)$ is continuous in $[-a, a]$ and

$$h(x) = \sum_1^n c_i \delta(x - x_i) \quad (26b)$$

The Fourier transform of $f(x)$ is given by

$$F(X) = G(X) + H(X) \quad (27a)$$

where, as is well-known from standard FT theory [6, 7, 8]

$$|G(X)| \text{ varies as } 1/X^l \text{ as } X \rightarrow \infty, \quad l \geq 1 \quad (27b)$$

while

$$H(X) = \sum_{j=1}^n c_j e^{i2\pi x_j X} \quad (27c)$$

has infinitely many oscillations of undying (r.m.s.) amplitude provided there are at least two δ -functions - see Appendix). Now,

$$\begin{aligned} |F(X)|^2 &= F(X) \overline{F(X)} \\ &= (G(X) + H(X)) \cdot (\overline{G(X)} + \overline{H(X)}) \\ &= |G(X)|^2 + H(X)\overline{G(X)} + G(X)\overline{H(X)} + |H(X)|^2 \end{aligned} \quad (28a)$$

In this, using (27b), we see that the first three terms tend to zero as $X \rightarrow \infty$, so that

$$|F(X)|^2 \text{ varies as } |H(X)|^2, \text{ as } X \rightarrow \infty \quad (28b)$$

Therefore, since $|H(X)|^2$ has infinitely many oscillations of undying mean amplitude as shown above, $|F(X)|^2$ also has infinitely many oscillations. Also, the r.m.s. amplitude of the oscillations of $|F(X)|$ are of undying magnitude.

b) Discontinuous functions.

Since discontinuities in a function lead to δ -functions

in its derivative, using the above considerations, we can conclude that if the function $f(x)$ has two, or more, discontinuities, then the absolute value of the Fourier transform of its derivative will have infinite oscillations. But, as discussed in (d) of Section 3, the Fourier transform (say $F_1(X)$) of the derivative, namely $f^{(1)}(x)$, is just the product of $(-2\pi iX)$ and the Fourier transform $F(X)$ of the function $f(x)$. Hence we deduce that $|F(X)|$, given by

$$|F(X)| = |F_1(X)| / 2\pi |X| \quad (29)$$

will also have infinitely many oscillations. The argument is that, in $|F_1(X)|$, the part $G_1(X)$ due to the piecewise continuous parts $g^{(1)}(x)$ of the derivative $f^{(1)}(x)$ will die off as $1/|X|$ as $|X| \rightarrow \infty$, while the FT $H_1(X)$ of the δ -function components $h^{(1)}(x)$ in

$$f^{(1)}(x) = g^{(1)}(x) + h^{(1)}(x) \quad (30)$$

will continue to have oscillations of undying root mean square amplitude as $|X| \rightarrow \infty$. Hence, in

$$F_1(X) = G_1(X) + H_1(X) \quad (31)$$

$|G_1(X)| \rightarrow 0$ as $|X| \rightarrow \infty$, while $\langle H_1(X) \rangle^2 \stackrel{1}{\rightarrow}$ is a constant s_1 , as $|X| \rightarrow \infty$. Hence in (24), these latter oscillations survive, although the amplitude will die off as $1/|X|$, as $|X| \rightarrow \infty$.

(c) Function and first derivative continuous but a higher Derivative discontinuous at two points.

In the case in which the first derivative is continuous, but the second is discontinuous, we have analogous to Eq.(25),

$$f^{(2)}(x) = g^{(2)}(x) + h^{(2)}(x) \quad (32)$$

and exactly the same situation as in Eq.(26) holds for its Fourier transform $F_2(X)$.

$$F_2(X) = G_2(X) + H_2(X) \quad (33)$$

where

$$|G_2(X)| \rightarrow 0, \langle |H_2(X)|^2 \rangle \rightarrow s_2, \text{ as } |X| \rightarrow \infty \quad (34)$$

Hence, analogous to (24), we have, for the Fourier transform of the original function $f(x)$,

$$|F(X)| = |F_2(X)| / 4 \pi^2 X^2 \quad (35)$$

in which the infinite number of oscillations in $H_2(X)$ survive,

although with the root mean square amplitude decays as $1/X^2$.

In this way, if the function $f(x)$ and all its derivatives of order upto $(j - 1)$ are continuous, and the j th derivative is discontinuous at least at two points, then it follows that $|F(X)|$ will have an infinite number of oscillations, but with amplitudes falling off as $1/|X|^j$. This result is valid for all j , however large.

Hence, absence of infinite oscillations can occur, if at all, only for functions $f(x)$ for which $f^{(j)}(x)$ does not contain two δ -functions for all j . (We shall discuss the precise consequence of this condition in the Appendix).

6. Infinitely differentiable functions of bounded support

(a) General Remarks

If the function $f(x)$ is defined to have non-zero values only between $x = -a$ and $+a$ (as generally assumed in this report), we shall consider the special case where the function is infinitely

differentiable within this bounded support. As a simple example, we may take the following function:

$$f(x) = \frac{\sin \pi bx}{\pi x}, \quad \text{for } -a \leq x \leq a \quad (36)$$

$$f(x) = 0, \quad \text{elsewhere}$$

The idea is quite simple. An infinitely differentiable function of the type $f(x)$ is the inverse Fourier transform of a function $F(X)$ of BS, and it extends from $-\infty$ to $+\infty$. Now, if this $f(x)$ is cut off below $-a$ and above $+a$ so as to have a bounded support, we wish to investigate what happens to its Fourier transform $F(X)$. We shall show below, quite generally, that the function $F(X)$ (which is naturally ID) is also infinitely oscillating.

If, in the discussion of the last para, the space of the original function $f(x)$ and of the Fourier transform $F(X)$ are interchanged, then we find that this problem is extremely relevant to physics, and diffraction theory in general, and for the theory of reconstruction of an object from its diffraction pattern. Thus if $f(x)$ is a function of bounded support (as is

true of a molecule in crystallography, or of any finite object which is diffracting in physics) then its Fourier transform $F(X)$ has unbounded support (UBS). This is a well-known fact, namely that any finite object has a diffraction pattern extending right upto infinity (though it is not stated so categorically in books on Optics - [9] [13] - and Crystallography - [4] [10].) The problem of the reconstruction of the original object from the diffraction pattern, or its Fourier transform, then becomes an interesting problem. This is an exceedingly important topic, since it is used not only in x-ray crystallography and optical diffraction, as in holograms, but it is also very widely used for image reconstruction or pattern recognition. It has also relevance to NMR and IR spectrographs [11], [12], where Fourier-transform instruments for recording the spectrum have a very much greater power than the direct way of measuring the lines in it.

In all these cases, the Fourier transform cannot be measured upto $|X| \rightarrow \infty$. Therefore $F(X)$ has to be cut off at some

maximum value X_1 for $|X|$. Under these conditions, the interesting result that we have proved is that the object, reconstructed by inverse Fourier transformation, will have a tail of oscillating intensity, or density, that extends right upto infinity; and the number of oscillations is also infinite. This is a really beautiful result, which may be stated in words, as follows:

"If the diffraction pattern of a finite object ($f(x) = 0$, for $|x| > a$), which extends upto $|X| \rightarrow \infty$. is cut off beyond a finite range $\pm X_1$, then the reconstructed object extends upto infinity in x , instead of being limited to the finite space that the original object occupied, and this reconstructed object has infinitely many oscillations".

The words "function $f(x)$ " and "Fourier transform $F(X)$ " can be interchanged in what has been said above as these two have a reciprocal relationship. We know from the previous study that, if either one of them is of BS, then the other one is ID. If the

latter is cut off outside a range so as to have BS, the former, on reconstruction, has an infinite number of oscillations extending to infinity. This means that, in any practical problem, image reconstruction via the Fourier transform method, can never be perfect.

(b) Proofs of the results.

Consider a function $f(x)$ which is ID, and take a section of it, of BS, between $-a$ and $+a$, which we denote by $\phi(x)$. Then

$$\phi(x) = f(x) \quad \text{for } -a < x < a \\ (37)$$

$$\phi(x) = 0 \quad \text{elsewhere}$$

We wish to examine the properties of its F.T., which we denote by $\Phi(X)$. Then

$$\Phi(X) = \int_{-\infty}^{+\infty} \phi(x) e^{i2\pi X x} dx \quad (38a)$$

$$= \int_{-a}^{+a} f(x) e^{i2\pi X x} dx \quad (38b)$$

(i) Even (real) function $f(x)$.

To start with, suppose $f(x)$ is even, i.e.

$$f(-x) = f(x) \quad (39a)$$

Then;

$$f^{(2j)}(-x) = f^{(2j)}(x) \text{ and } f^{(2j+1)}(-x) = -f^{(2j+1)}(x) \quad (39b)$$

Thus, (38) becomes

$$\tilde{\Phi}(X) = 2 \int_0^a f(x) \cos 2\pi X x \, dx \quad (40)$$

and, since the function $f(x)$ is ID, we can integrate it by parts and obtain, (for X large enough) a convergent series as follows:

$$\begin{aligned} \int_0^a f(x) \cos 2\pi X x \, dx &= \frac{1}{2\pi X} \left[f(x) \sin 2\pi X x \right]_0^a \\ &\quad - \frac{1}{2\pi X} \int_0^a f^{(1)}(x) \sin 2\pi X x \, dx \end{aligned} \quad (41a)$$

$$= \frac{f(a)}{2\pi X} \sin 2\pi a X + \frac{f^{(1)}(a)}{(2\pi X)^2} \cos 2\pi a X - \frac{f^{(2)}(a)}{(2\pi X)^3} \sin 2\pi a X - \dots \quad (41b)$$

Thus,

$$\begin{aligned} \tilde{\Phi}(X) &= 2 \sum_{j=0}^{\infty} (-1)^j \frac{f^{(2j)}(a)}{(2\pi X)^{2j+1}} \sin 2\pi a X \\ &\quad + 2 \sum_{j=0}^{\infty} (-1)^j \frac{f^{(2j+1)}(a)}{(2\pi X)^{2j+2}} \cos 2\pi a X \end{aligned} \quad (42a)$$

$$= A(X) \sin 2\pi a X + B(X) \cos 2\pi a X \quad (42b)$$

From the condition of ID for $f(x)$, we know that $|f^{(j)}(x)| \leq Kc^j$.

Hence, if $|X|$ is made large enough, we can show that, if $f^{(0)}(a)$ and $f^{(1)}(a)$ are non-zero,

$$A(X) = \frac{2f^{(0)}(a)}{2\pi X} + O\left[\frac{1}{(2\pi X)^2}\right] \quad (43a)$$

and

$$B(X) = \frac{2f^{(1)}(a)}{(2\pi X)^2} + O\left[\frac{1}{(2\pi X)^3}\right] \quad (43b)$$

$$= O\left[\frac{1}{(2\pi X)^2}\right] \quad (43c)$$

Hence, there is a leading term $f^{(0)}(a)/\pi X$, relative to which all the other terms are negligible, being $O(1/(2\pi X)^2)$, for $|X|$ large enough. Therefore, as $|X|$ becomes larger and larger, the succeeding terms become more and more insignificant, so that

$$\Phi(X) \approx \frac{f^{(0)}(a)}{\pi X} \sin 2\pi ax \quad (44)$$

whose oscillations form the predominant feature of $\Phi(X)$. (This can obviously be generalized to the case where $f^{(0)}(a) = 0$,

$f^{(1)}(a) = 0, \dots, f^{(k-1)}(a) = 0$, so long as some derivative $f^{(k)}(a)$ is non-zero for $x = \pm a$).

(ii) Odd (real) function $f(x)$.

In this case, we have

$$f(-x) = -f(x) \quad (45a)$$

and

$$f^{(2j)}(-x) = -f^{(2j)}(x), \quad f^{(2j+1)}(-x) = +f^{(2j+1)}(x) \quad (45b)$$

so that (38) becomes

$$\underline{\Phi}(x) = 2 \int_0^a f(x) \sin 2\pi x dx \quad (46)$$

which, on integrating by parts, takes a form similar to (41b), namely

$$\begin{aligned} \int_0^a f(x) \sin 2\pi x dx &= -\frac{f(a) \cos 2\pi a x}{2\pi x} + \frac{f'(a) \sin 2\pi a x}{(2\pi x)^2} \\ &\quad + \dots \end{aligned} \quad (47)$$

Following the same argument as for even functions, this also has a leading term, with respect to which, the sum of all other terms is insignificant as $|X|$ becomes large enough. Hence,

$$\underline{\Phi}(x) \approx \frac{2if^{(k)}(a)}{(2\pi x)^{k+1}} \sin 2\pi a x + O\left(\frac{1}{(2\pi x)^{k+2}}\right) \quad (48)$$

and the value of $\underline{\Phi}(x)$ is infinitely oscillatory.

(iii) General (real) function.

If the function $f(x)$ is neither even nor odd, it can be expressed as the sum of an even function $g(x)$ and an odd

function $h(x)$ as :

$$f(x) = g(x) + h(x) \quad (49a)$$

with

$$g^{(j)}(-x) = (-1)^j g^{(j)}(x), \quad h^{(j)}(-x) = (-1)^{j-1} h^{(j)}(x) \quad (49b)$$

Hence, the discussion in the previous subsections (i) and (ii) are both applicable, and the leading term in $\Phi(x)$ of (38) is one of three types :

$$\Phi(x) = A_k (2\pi x)^{-k} \cos 2\pi ax \quad (50a)$$

$$\text{or} \quad = B_k (2\pi x)^{-k} \sin 2\pi ax \quad (50b)$$

$$\text{or} \quad = (2\pi x)^{-k} [A_k \cos 2\pi ax + i B_k \sin 2\pi ax] \quad (50c)$$

where A_k, B_k may be complex. In all cases, except when $B_k = A_k$ in (50c). $\Phi(x)$ can be shown to be infinitely oscillatory for sufficiently large values of $|x|$. In that special case, in which $A_k = B_k$ for the smallest value of k , we obtain

$$\Phi(x) = (2\pi x)^{-k} A_k e^{i2\pi x} \quad (51a)$$

leading to a non-oscillatory function $A_k (2\pi x)^{-k}$ for $|\Phi_k|$, as $x \rightarrow \infty$. However in such a case, there will be some k' , for

which $A_k \neq B_k$, and this term for k' will have the form :

$$\tilde{\phi}(x) = (2\pi x)^{-k'} c_{r_1} \cos(2\pi a x + \delta) \quad (51b)$$

which is obviously oscillatory.

(iv) General complex function

The extension of these considerations to the case when function is complex and it is neither even and odd, can be obtained, if required, from the results in subsections (i), (ii) and (iii). However, it is not discussed here, since the general proof given in Section 7 covers this case as well.

7. Analytic functions of bounded support

As seen from the results in Section 5, no proof is needed for the case, where a function $f(x)$ is analytic (but not ID) from $-a$ to $+a$, and zero outside, provided the function, or any derivative $f^{(j)}(x)$ is discontinuous at $x = -a$ and $+a$, but is analytic within this bounded support. So, we are left only with the case where $f(x)$ has the following properties :

(i) $f(x)$ is analytic, but not ID, for $-a \leq x \leq +a$ ($=f_1(x)$, say), and $f'(x) = 0$ for all $x \in [-a, +a]$ and from $x = a$ up to ∞ ($=f_2(x)$, say).

(ii) The function and all its derivatives $f^{(j)}(x)$ are continuous at $x = \pm a$, i.e.,

$$f_2(-a_-) = f_1(-a_+) = 0, \text{ and } f_1(a_-) = f_2(a_+) = 0 \quad (52a)$$

and

$$f_2^{(j)}(-a_-) = f_1^{(j)}(-a_+) = 0, \text{ and } f_1^{(j)}(a_-) = 0, \text{ for all } j. \quad (52b)$$

but

$$\lim_{j \rightarrow \infty} f_1^{(j)}(x) \neq \text{finite for } -a < x < a \quad (52c)$$

which means that

$$\lim_{j \rightarrow \infty} f_2^{(j)}(x) \neq f_1^{(j)}(x) \text{ at } x = \pm a \quad (52d)$$

Under these conditions, the proofs given in Section 6, for ID functions, cannot be applied. However, when the Fourier transform $F(X)$ of a typical function of the above type, namely

$f(x) = e^{-1/(a^2-x^2)}$ was evaluated by numerical integration, it

was found to have oscillations of approximate period $1/a$. Hence it appears that the proof of IO for this case must be obtained as part of a general result of the following type:

$$\text{"If } F(X) \text{ is ID, then it is IO"} \quad (53)$$

Once this result is proved generally, then it covers all the cases discussed previously in this report, namely when $F(X)$ is the F.T. of a function $f(x)$, of BS and AI. This is because we already know, from Matphil Reports Nos. 14 and 15, that "If $f(x)$ is of BS, then $F(X)$ is ID". Of course, as mentioned in Section 2, we always assume that $f(x)$ is AI, so that $F(X)$ is bounded in magnitude and is continuous for all X . We also have an additional property that $F(X) \rightarrow 0$ as $X \rightarrow \infty$. (This latter property is violated if $f(x)$ consists of at least two δ -functions, but in this case, $F(X)$ is demonstrably IO, and it need not be considered.)

(a) Preview of steps in the general proof of (53)

However, the proof of (53) with this extent of generality

seems to be not possible if only the techniques considered earlier in this report are employed. Since $f(x)$ is NID, $f^{(j)}(x)/j!$ may not converge as $j \rightarrow \infty$, so that the methods making use of Taylor expansion, or partial integration, (carried out infinitely many times) do not work. Hence we shall employ a completely different approach to deal with this case. We shall prove (53) by proving its equivalent "reverse" (contrapositive) form:

$$\text{"If } F(X) \text{ is NI0, then it is NID"} \quad (53a)$$

Since we know from the previous study that

$$\text{"If } f(x) \text{ is of UBS, then } F(X) \text{ is NID"} \quad (54)$$

it will be sufficient to prove (55) :

$$\begin{aligned} &\text{"If } F(X) \text{ is NI0, then its inverse F.T. } (ff(x)) \text{ has UBS"} \\ &\quad (55) \end{aligned}$$

in order to obtain the result (53) as a consequence. Actually, if $F(X)$ is the F.T. of $f(x)$ which is both BS and AI, then (55) itself leads to the contradiction that

" $f(x)$ is BS $\Rightarrow f^2(x)$ is UBS, if in addition, $F(X)$ is NI0" (56)

We shall prove (56) under quite general conditions. First we prove it for the case when $f(x)$ is real and even function of x . Then we use this to prove the corresponding results in the case when $f(x)$ is real and odd and for the case where $f(x)$ is real and general. (neither necessarily even nor odd). In all these cases we show that $F(X)$ is IO, in the sense that it has infinite number of oscillations for values of X extending to both $+\infty$ and $-\infty$.

However, in the still more general case of $f(x)$ being complex (and general in the above sense) we find that the full proof is not readily possible. We shall prove that $F(X)$ is partially infinitely oscillatory (PIO) in the sense that there are an infinite number of oscillations either for values of X extending towards $+\infty$, or extending towards $-\infty$. The proof is not complete in showing that the oscillations exists on both sides (IO), although very likely this may be the case when $F(X)$ is the Fourier Transform

of a general function $f(x)$.

(b) Even (real) function $f(x)$

We shall prove (56) for this case as follows. Suppose that $F(X)$ has only a finite number of maxima and minima (i.e., that it is NIO). Then, we can always find a number X_1 , such that all the maxima and minima of $F(X)$ are contained in the interval $[-X_1, +X_1]$. Outside this interval (above X_1 and below $-X_1$), $F(X)$ must be monotonic. We then modify the function $F(X)$ to be a function $H(X)$ which is monotonically decreasing from the origin to infinity, by taking the function $H(X)$ to be same as $F(X)$ from $-\infty$ to $-X_1$ and from $+X_1$ to $+\infty$ and making it equal to the infinitely differentiable function $M(\sin \pi l x)/\pi X$, from $-X_1$ to $+X_1$, so that it is continuous at $-X_1$ and $+X_1$, and making $H(X)$ monotonically decreasing from 0 to $+X_1$ and $-X_1$, by choosing M and l suitably.

We then show that this monotonically decreasing F.T. leads by inverse Fourier transformation to a function $h(x)$ that has

unbounded support, and non-zero for all x . We also show that the difference between the two function $H(X)$ and $F(X)$ for the interval between $-X_1$ and $+X_1$, is infinitely differentiable, so that its inverse F.T. also has unbounded support and an infinite number of zeros, as per Section 6. In this way, we prove that $ff(x)$ is UBS, as in (56), and we can deduce from the contradiction in it that $F(X)$ cannot be NIO, if $f(x)$, which is BS and AI, is in addition real and even.

We shall first prove result (56) in a rather restricted form (57) below.

"If $F(X)$ is an even function, and if it decreases monotonically from its maximum value at $X=0$, to $X=\infty$, as well as to $X=-\infty$, then its inverse F.T. $ff(x)$ has UBS" (57)

It may be noted that $F(X)$ is also even and real.

We know that $ff(x)$, the inverse F.T. of $F(X)$ is given by

$$\begin{aligned} ff(x) &= \int_{-\infty}^{+\infty} F(X) e^{-i2\pi X} dX \\ &= 2 \int_0^{\infty} F(X) \cos 2\pi X dX \end{aligned} \quad (58)$$

Let M be the maximum value of $F(X)$, and let

$$F(X) = H(X) - G(X) \quad (58a)$$

where $H(X) = M$ (58b)

and $G(X) = M - F(X)$ (58c)

Then $G(X)$ increases monotonically from $X = 0$ to $X = \pm \infty$, as shown in Fig.1. The product of $G(X)$ with $\cos 2\pi x X$ is also shown in the figure, for the intervals of $2\pi x X$ from 0 to $\pi/2$, $\pi/2$ to $3\pi/2$, $3\pi/2$ to $5\pi/2$, . . . , which are denoted by the indices $1, 2, 3, \dots$,

Fig.1. The function $F(X)$, $H(X) = M$, and $G(X) = M - F(X)$. The product $F(X) \cos 2\pi x X$ is shown by the wavy line, and the shaded negative area (integral), I_{2k} , is seen to be larger in extent than the previous unshaded one, I_{2k-1} , for all k .

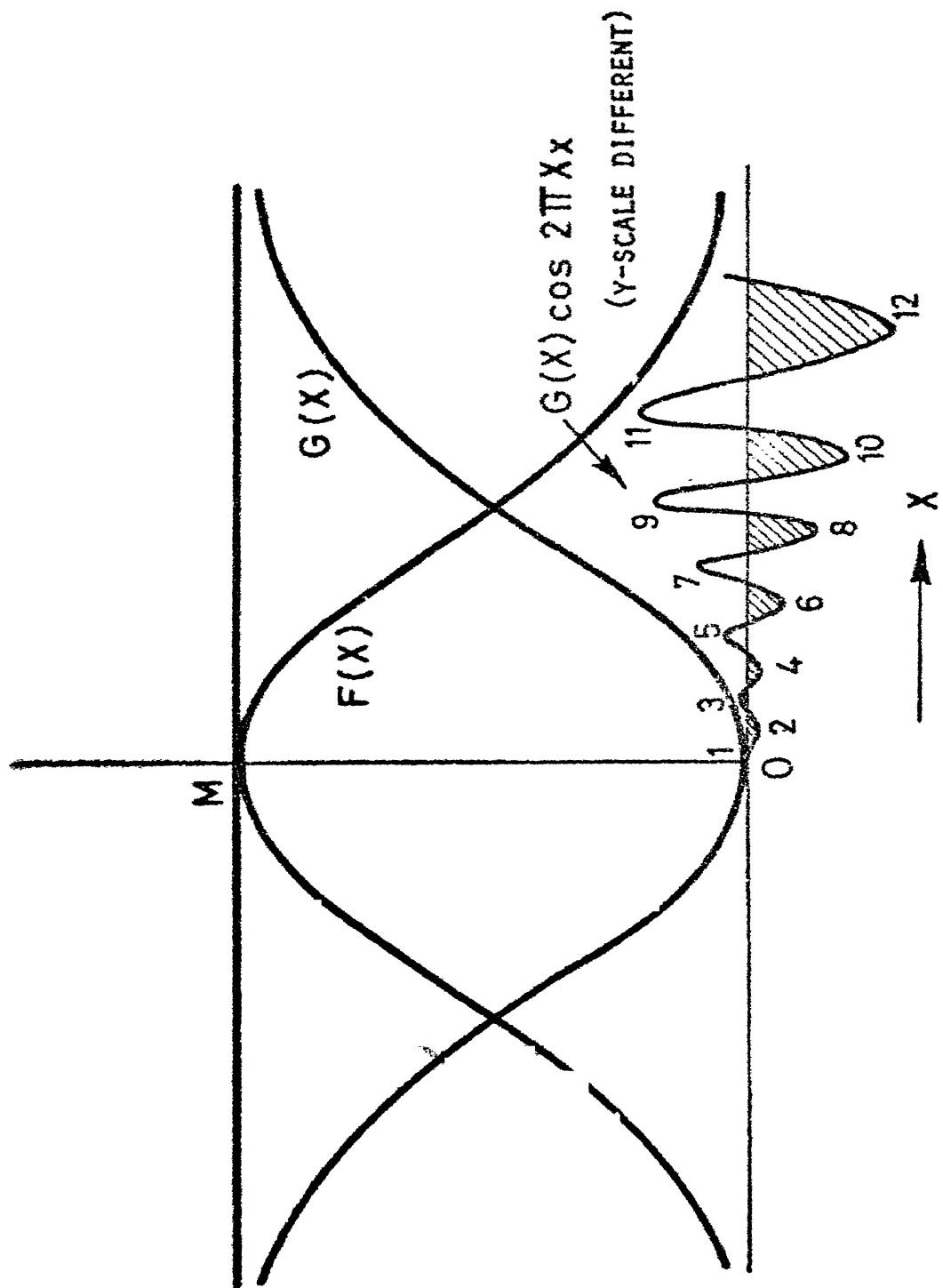
Then, the integral is

$$I = \int_0^{\infty} G(X) \cos 2\pi x X dX = (I_1 - I_2) + (I_3 - I_4) + \dots \quad (59a)$$

where the contributions from each of these intervals, namely I_1 , I_2 , I_3 etc, have the property that

$$I_1 < I_2 < I_3 < \dots < I_{2k-1} < I_{2k} < \dots \quad (59b)$$

This is because $G(X)$ is a continuously increasing function. Hence,



every one of the quantities $(I_1 - I_2)$, $(I_3 - I_4)$, . . . $(I_{2k-1} - I_{2k})$

. . . in (59a) is negative, so that

$$g(x) = 2I, \text{ is -ve, and } \neq 0, \text{ for all } x \quad (60)$$

From (58a), we obtain, by inverse Fourier transformation, the equation

$$\begin{aligned} ff(x) &= h(x) - g(x) \\ &= M \delta(x-0) - g(x) \end{aligned} \quad (61)$$

Since $\delta(x-0) = 0$ for $x \neq 0$, we get that

$$ff(x), = -g(x), \text{ is } \neq 0 \text{ for all } x \neq 0 \quad (62)$$

Hence $ff(x)$ has unbounded support (UBS) and (57) is proved.

(c) Even real function $f(x)$ with $F(X)$ having a finite number of maxima and minima

We shall now prove (56) in a somewhat more general form (63), making use of (57) :

"If $f(x)$ is a real even function, and its F.T. $F(X)$ is NIO, such that its minima are contained in $[-x_1, x_1]$, and if $F(X)$ decreases monotonically from $X = x_1$ to $X = \infty$ (and from

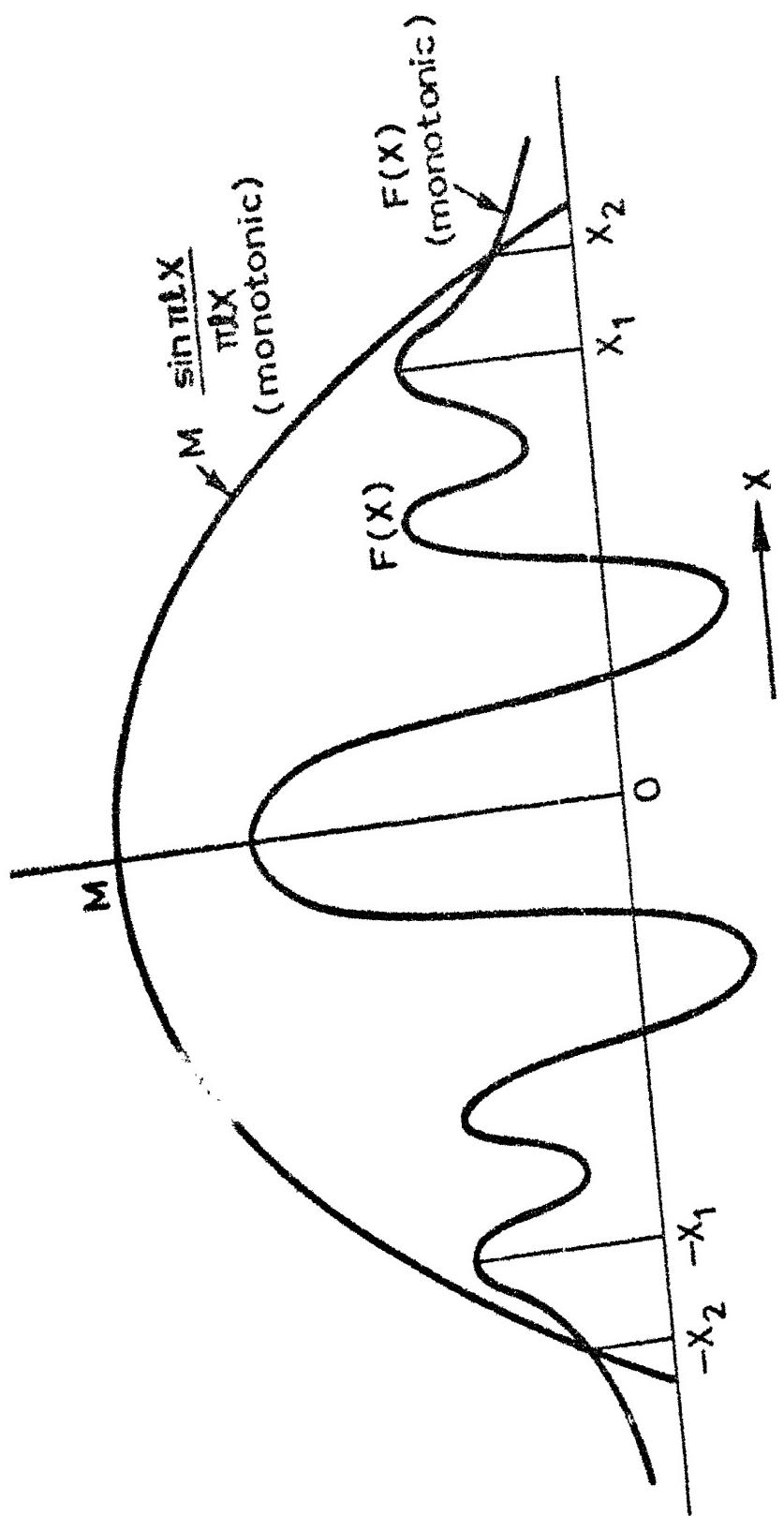
$X = -X_1$ to $X = -\infty$), then its inverse F.T. $\text{ff}(x)$ has UBS" (63)

Let M be larger than the maximum value of $F(X)$ for $X = -\infty$ to $X = +\infty$. We know that the function $M(\sin \pi l X)/\pi X$ has a maximum at $X = 0$, and decreases monotonically from $X = 0$ to its first minimum as $X = 1/l$. Since $F(X)$ decreases monotonically for $|X| > X_1$, we can choose l small enough in such a way that $F(X)$ and $M(\sin \pi l X)/\pi X$ intersect at $\pm X_2$, with $|X_2| > |X_1|$, as shown in Fig.2. Also, since $f(x)$ is real and even, (with BS and AI), $F(X)$ is necessarily ID for all X , and is real and even.

Fig.2. A real even function $F(X)$ with a finite number of maxima and minima, along with the function $M(\sin \pi l X)/\pi X$ from $-X_2$ to X_2 . Note that $G(X)$, of text, is a continuous and monotonically decreasing from $X = 0$, to $X = \infty$ and to $X = -\infty$.

Now, define two functions $G(X)$ and $H(X)$ as follows;

$$\begin{aligned} G(X) &= M(\sin \pi l X)/\pi X, \quad -X_2 \leq X \leq X_2 \\ &= F(X), \quad \text{otherwise} \end{aligned} \tag{64a}$$



and

$$\begin{aligned} H(X) &= F(X) - M(\sin \pi l X) / \pi X, \quad -X_2 \leq X \leq X_2 \\ &= 0, \quad \text{otherwise} \end{aligned} \quad (64b)$$

Since $G(X)$ is a real even function with only one maximum at $X=0$, it follows from the previous subsection, that

$$g(x) = \left[\text{Inverse F.T. of } G(X) \right] > 0, \quad \text{for all } x \neq 0 \quad (65a)$$

As regards $H(X)$, $F(X)$ in (64b) is necessarily ID since $F(x)$ is BS and AI. Since, the sinc function, $M(\sin \pi l X) / \pi X$, is also ID, $H(X)$ of (64b) is ID for $-X_2 \leq X \leq X_2$, and zero outside this bounded support, and it is also real and even. Hence, by the results in Section 6(b)(i), the inverse F.T. of $H(X)$, namely $h(x)$ has the following properties:

$$\begin{aligned} h(x) &\text{ is ID, has UBS, and is IO,} \\ &\text{with an infinite number of zeros} \end{aligned} \quad (65b)$$

Consequently , the sum $gg(x) + hh(x)$ has non-zero values for $|X|$ greater than any chosen $|x_1|$, however large. Therefore,

$$ff(x) = gg(x) + hh(x) \text{ has UBS} \quad (66)$$

where $ff(x)$ is the inverse F.T. of $F(X) = G(X) + H(X)$. This proves (63), which is in contradiction with the assumption that $f(x)$ has BS.

In effect, we have shown that, for any real even $f(x)$, (of BS and AI), its F.T. ($F(X)$) is infinitely oscillatory (IO), since an assumption of NIO leads to the contradiction that $f(x)$ has BS, while $ff(x)$ ($=f(x)$) has UBS.

(d) Odd real function $f(x)$ with $F(X)$ being NIO

If we have an odd function such that $f(-x) = -f(x)$, then it follows that its Fourier transform is purely imaginary and is given by

$$F(X) = 2i \int_0^{\infty} f(x) \sin 2\pi x X dx \quad (66)$$

Unfortunately, it is not possible to prove that the assumption of NIO for this case will lead to UBS for $ff(x)$. However, this can be got over by considering the square of $F(X)$, namely $(F^2(X))$, which is necessarily positive and has the property of being even. Hence by the previous section $F^2(X)$ is IO, and therefore $F(X)$ is IO.

Thus, without much difficulty we have shown that an odd function is also infinitely oscillatory and has an infinite number of maxima and minima both towards $X = +\infty$, and towards $X = -\infty$.

(e) General real function $f(x)$

We shall now prove (56) for a function $f(x)$, which is real but not necessarily even. Then, its Patterson (autocorrelation) function $p(x)$ defined by

$$p(x) = \int_{-\infty}^{+\infty} f(y) f(x+y) dy \quad (67)$$

is real and even, and also has BS. Now, the F.T. of $p(x)$ is

$$P(X) = F(X) \bar{F}(-X) = |F(X)|^2 \quad (68a)$$

since

$$\text{for a real } f(x), \bar{F}(-X) = \bar{F}(X) \quad (68b)$$

the condition that the $|F(X)|$ is NIO, is equivalent to $|F(X)|^2$ being NIO, or the even function $P(X)$ being NIO, which is impossible, since it leads to $p(x)$ ($= p(x)$) being of UBS, by (63). Hence, the contradiction (56) is proved for a general real function $f(x)$, and we deduce there from that

"If $f(x)$ is real and of BS, but not necessarily even, then $F(X)$ is IO" (69)

(f) General complex function $f(x)$

In this case, $f(x)$ is any general complex function, and further the equality $\bar{F}(-X) = \bar{F}(X)$, which occurs for a real function $f(x)$, is no longer valid. Consequently, the proof has to take a round about route. Since $f(x)$ is complex, we write it in the form

$$f(x) = f_1(x) + i f_2(x) \quad (70)$$

in which both $f_1(x)$ and $f_2(x)$ are real functions, not necessarily either even or odd. We now take the Fourier transform of $f(x)$ by finding the F.T. of $f_1(x)$ and $f_2(x)$ individually and taking into account the linear equation (70). If we denote

$$\text{F.T. of } f_1(x) = A_1(X) + iB_1(X) \quad (71a)$$

$$\text{F.T. of } f_2(x) = A_2(X) + iB_2(X) \quad (71b)$$

then it follows that

$$F(X) = [A_1(X) - B_2(X)] + i[A_2(X) + B_1(X)] \quad (72)$$

Omitting the variable X throughout, we obtain from (72) that the square of the magnitude of $F(X)$ is $|F(X)|^2$ given by (73) below:

$$|F(X)|^2 = A_1^2 + B_1^2 + A_2^2 + B_2^2 - 2(A_1B_2 - A_2B_1) \quad (73)$$

It also follows that

$$F_1(-X) = A_1(X) - iB_1(X) \quad (74a)$$

$$F_2(-X) = A_2(X) - iB_2(X) \quad (74b)$$

From which the square of the magnitude of $F(-X) = F_1(-X) + iF_2(-X)$ becomes

$$|F(-X)|^2 = A_1^2 + B_1^2 + A_2^2 + B_2^2 + 2(A_1B_2 - A_2B_1) \quad (75)$$

It is readily seen from (73) and (75) that $|F(X)|^2$ is a

real function, which is expressible in terms of an odd part and an even part as below:

$$|F(X)|^2 = G(X) - H(X) \quad (76a)$$

$$\begin{aligned} |F(-X)|^2 &= G(-X) + H(-X) \\ &= G(X) + H(X) \end{aligned} \quad (76b)$$

Hence $G(X)$ is a symmetric function and $H(X)$ is antisymmetric (odd) function of X . As was shown in Sec. (b) and (d), both of these are infinitely oscillatory. However, there seems to be no simple theorem to find out whether the sum of two infinitely oscillatory functions is itself IO or not. However, in this case, it is obvious that both $G(X) + H(X)$ and $G(X) - H(X)$ cannot be NIO for the range 0 to ∞ of X , because this would mean that the oscillations of $G(X)$ and $H(X)$ are nearly opposite in phase in one of the two cases. Then, it necessarily means that they will be in phase for the other, which will therefore be oscillatory. Hence, we come to the conclusion that $|F(X)|^2$ is definitely PIO (partially infinitely oscillatory), by which is meant the fact that it has a infinite number of oscillations either from 0 to ∞ or from 0 to $-\infty$ (or both).

This seems to be the best result that can be obtained in this case, although it seems very likely that $F(X)$ would be IO for both positive and negative values of X , since the functions $G(X)$ and $H(X)$ are not independent, as will be seen by an examination of equations (73) and (75), in which both are seen to be functions of A_1 , B_1 , A_2 and B_2 . However, so far it has not been possible to prove this wider result. Therefore, we leave this problem at this stage with the general results being as follows:

1. If $f(x)$ is real, BS and AI, then $F(X)$ is UBS, ID and IO
2. If $f(x)$ is complex, BS and AI, then $F(X)$ is UBS, ID and PIO.

8. Comments and Conclusions

(a) Resume of the proof

We will briefly summarize in this section the main results obtained in this study, along with the essential steps in the proof, and also some possible applications of these results. The essential outcome of this study is the fact that the F.T. of a physical function is infinitely oscillatory, as stated at the beginning of Section 3, and proved in Section 7. The steps by which the complete proof is obtained may be summarized as follows:

1. Premise 1: The theorem has as its premise that the function $f(x)$ is AI and is of BS (which is true for all functions $f(x)$ considered in this report). This leads to its F.T., $F(X)$, being of UBS and ID.

2. Special conditions under which $F(X)$ is IO are :

- (a) If $f(x)$ contains at least two δ -functions, then $F(X)$ is IO, of undying r.m.s. amplitude.
- (b) If $f^{(j)}(x)$ contains at least two δ -functions (for j - any finite

integ. r), then $F(X)$ is IO, but the amplitude of the oscillations is $O(1/X^{j+1})$, and decays to zero as

$X \rightarrow \infty$.

3. General proof when 2(a), (b) are not true, and $f(x)$ is analytic, but not ID, requires several steps. First, we prove

(a) Result 1: If $f(x)$ is real and even, and is ID in addition in its bounded support, then $F(X)$ is IO. (Sec. 6).

Then, we start with an $f(x)$ (which is AI and BS, as per Premise 1), and suppose, if possible, that its F.T. $F(X)$ is NIO * We then show that the inverse F.T. of $F(X)$, namely $ff(x)$, has UBS, contrary to the starting assumption that $f(x)$ has BS, so that it follows that $F(X)$ is IO. This proof requires Result 1 for its construction. Thus, we obtain Result 2 below, without the restricting condition of ID on $f(x)$:

(b) Result 2: If $f(x)$ is real and even then its F.T., viz. $F(X)$, is IO, and $F(X)$ is also real and even.

We then generalize Result 2 to the following two Results 3 and 4:

(c) Result 3: If $f(x)$ is real and odd, then $F(X)$ is IO, $F(X) =$ a constant is excluded, as it is taken to be IO in this study (see p. 23).

and $F(X)$ is also real odd.

- (d) Result 4: If $f(x)$ is real, then $F(X)$ is complex, in general; but always $|F(-X)| = |F(X)|$, and $|F(X)|$ is IO.

Thereafter, we consider the most general case, namely when $f(x)$ is complex, and not necessarily even or odd. We show that $|F(X)|^2$ in this case can be expressed as $G(X) + H(X)$, where $G(X)$ and $H(X)$ are both real, and $G(X)$ is even and $H(X)$ is odd. Since each is IO, with oscillations extending upto $\pm\infty$, we obtain the following Result 5, which is less powerful than the previous four results:

- (e) Result 5: If $f(x)$ is complex, $|F(X)|$ is partially infinitely oscillatory (PIO), i.e. it has an infinite number of oscillations either from 0 to ∞ , or from 0 to $-\infty$.

In this last form, the possibility of IO, with oscillations on both sides, extending to $\pm\infty$, is not excluded. It is quite likely, but has not been proved. (See addendum, where IO for the Result 5 is indicated.)

(b) Comments regarding physical applications

In formulating the proofs in this report, the senior author's familiarity with optics and x-ray crystallography was found useful, and several well-known results in these fields formed the stimuli for the methods of approach adopted herein. Thus, it is well known that a function $f(x)$ representing the physical property of a finite body always has an F.T. which is of bounded variation and continuous (See Ref. 13, p.6). In our studies, we have proved, in addition, that this F.T., which extends from $-\infty$ to $+\infty$ of X, has also the property of being infinitely differentiable, and contains an infinite number of oscillations of $|F(X)|$

In fact, in proving the last result for the most general case, Eq. (72) was deduced following the derivation of the structure factor of a crystal exhibiting the property of anomalous dispersion (see Ref. 4, p.192, Eqs.(30a) and (30b)). Even Eq. (68b), for a general real function, is equivalent to Friedel's Law in crystallography (Ref. 4, p.168), which is violated when $f(x)$ is complex and

non-symmetric.

It is interesting that the whole report hinges on result⁺ which can be proved only if $f(x)$ is ID within its BS, for otherwise the series, obtained by repeated partial integrations, will not converge.

The most interesting consequence of the present report is that, if the F.T. of a physical function is truncated, and the function reconstructed by Fourier inversion, then the reconstructed image always has an infinite number of ripples. The ripples could be reduced in amplitude by suitable techniques, but they cannot be eliminated altogether.

It is interesting that all the results reported in this paper also hold for a square-integrable function ($f(x) \in L^2$) of an object of finite dimensions (i.e. having BS). This is so because, in these circumstances, L^2 implies L^1 , i.e. AI. The only additional property that we obtain is that the F.T. is also square integrable. However, if $f(x)$ has BS, $F(X)$ still has UBS, and extends right

throughout from $-\infty$ to $+\infty$. Also, mere AI and BS for $f(x)$, with no analyticity conditions, demands analyticity and TD for $F(v)$ for all points X from $-\infty$ to $+\infty$. The F.T. is also infinitely oscillatory. These results will be of great interest in the general theory of quantum mechanics.

Addendum 1

As mentioned in the preface, some new results have been obtained after the above studies had been completed, indicating that $F(X)$ is always IO, if $f(x)$ is analytic within the interval $x = -a$ to $+a$. Further, $F(X)$ is either IO or NIO, but cannot be PIO. Hence Result 5 can be improved from PIO to IO, thus making the main result of the report universally valid.

Addendum 2

The fact, that the oscillations for $X \rightarrow \infty$ have a period $\Delta X = 1/2a$, can be generalized for 2-D and 3-D Fourier transforms, by using F.T. formulae analogous to those used in the F.T. theory of tomography. This is reserved for a future report.

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PHILOSOPHY
OF
SCIENCE AND RELIGION

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(Presidential Address to a Symposium at the Centre for the
Study of World Religions, Dharmaram Pontifical
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(Presidential address to the symposium at Dharmaram Pontifical Institute of Theology and Philosophy Bangalore 29).

1. Introduction:

Although I am the head of a Department of Mathematical Philosophy, my contacts with philosophical thoughts have been only obtained from wellknown books like "The Story of Philosophy" by Will Durant, and the writings on Hindu Philosophy by Radhakrishnan. Therefore, when I comment on orthodox philosophy I have often tried to get the apt quotation from the writings of some wellknown philosopher to illustrate the points. I hope this will be excused, since my own personal knowledge of this subject is not sufficiently profound.

On the other hand, I have been a scientist all my life, and, in particular, I have devoted myself to research and original investigations ever since the early 40's. Therefore I can talk with some confidence on science, on the methods of science, on the attitudes and feelings of scientists about religious matters, and more generally, about the philosophy of science. In doing this, I shall try to give you a brief picture of what science is, and how scientists view the great problems imposed by religious concepts in the minds of everybody - problems such as "What is the nature of things?", "What force drives the Universe" and "What causes Order to exist in Nature?" and perhaps touch upon questions like — "Is what we see, and hear, and feel, the real nature of things, or is it only a view of these as seen by man?" In trying to understand such aspects of knowledge, science and philosophy mingle with one another. In fact the answers to many

of these questions have been given more than 2,000 years ago by philosophical thinkers of India, Greece and other places, although science has advanced into its full maturity only within the last century or so.

I should perhaps make an apology for taking up a subject of the above title for discussion, when I am myself not a specialist either in philosophy or religion. But I gain great courage from what a savant like Schroedinger has said about the need for a synthesis of all facets of life and knowledge, in his book, "What is Life?" He says "It has become next to impossible for a single mind to command more than a small specialised portion of it (knowledge). I can see no other escape from this dilemma than that some of us should venture to embark on a synthesis of facts and theory, albeit with second hand and incomplete knowledge of some of them — and at the risk of making fools of ourselves". If Prof. Schroedinger does not mind being considered a fool when he talks about biology from the point of view of a physicist, I also need not fear to talk about the synthesis of science with religion and philosophy, while I am a specialist only in science.

2. Definitions of Science, Philosophy and Religion

We shall start by defining briefly what are meant by the three fields of knowledge we have chosen to discuss. Considering science first, it is perhaps the most general of all methods of gaining knowledge. When man observes his outside surroundings, the land which he perceives, the heavens above with sun and stars which he sees in all its glory, and also

the panorama of living beings, and contemplates about them, he becomes a true scientist. Science consists in observing facts, in codifying them, in organising them, in explaining them, and in doing so, becoming able to produce new types of knowledge. Thus science consists of the acquisition of knowledge — in fact, science may be identified with Knowledge itself.

But, the philosophers would say that it is their duty to study the nature of Knowledge, and the Indian religious leaders would say that the highest form of religious experience is the merging of oneself with true Knowledge. Therefore, in the name of "knowledge", we can combine science, religion and philosophy. There is really nothing that one of them can explore, in the ultimate limit, that the other cannot.

However, when it comes to practicality, there is a distinction between the three. Science, we say, consists of the study of the external world by the mind of man. On the other hand, as Will Durand says, "philosophy considers the hazardous task of dealing with problems not yet open to the methods of science — problems like good and evil, beauty and ugliness, order and freedom, life and death; so soon as the field of inquiry yields knowledge, susceptible of exact formulation, it is called science".

On the other hand, if we go to aspects of our existence dealing with such subjects as the mode of life and conduct of man, it becomes part of religion. This field of study, namely ethics, is the study of ideal conduct; "the highest knowledge", said Socrates, "It is the knowledge of good and evil, the knowledge of the wisdom of life". In exactly the same manner, according to Ancient Indian scholars, philosophy is at no time unconnected with

with religion. The supreme objective of the true seeker after truth is, according to them, the ability to merge the Inner Being of man (Atman) with the Supreme Being (Brahman) that exists transcending every object in the Universe.

3. True Religious Spirit

When we talk about religion, there are two aspects — one inner and the other outer — the words inner and outer being used with respect to the human being. It is an interesting fact that almost all religions agree in prescribing the principles of good conduct and in specifying what "outer" processes and actions can lead to satisfaction, happiness and inner liberation. However, they all also agree in saying that it is not the actions alone that count, but that it is the thoughts behind these that is as important, if not more important, than the actions performed. Do we not find persons who will publicly announce large gifts to charitable agencies, but who in their own institutions, would refuse a small rise in the salary of their lowest servants? They surely do not have a charitable heart. True religion demands that one shall be completely of one heart, whether in action, in thought, or in meditation (*manasā vāchā karmāṇā*). In this connection, I am reminded of the words of Plato, as to the meaning of the word "justice" — "simply that each man shall receive the equivalent of what he produces and shall perform the function for which he is best fit. A just man is a man in just the right place and doing his best and giving the full equivalent of what he receives".

Justice and truth, when welded together, form the bedrock of a religious life. There is no other language in the world that has the exact word for it than our Sanskrit — the word is '*Dharma*' and it is appropriate that the organisers of this Institute have given it the name *Dharmaram*. If *dharma* is achieved, and if *dharma* is maintained, nothing more is needed for the world to be happy and free of injustice.

The organisers of this school have asked me to include in my talk a few comments on religion as it relates to man, and that is why I have treaded into this territory of pure religion and discussed about what true religious conduct is. As already mentioned, it is not enough that one gives away one's possessions to the poor people for him to go to heaven. That charity must come from the heart; and if the heart is there in full, what is offered, or how little is offered, is of little matter. In fact, Samkarācārya puts this in the pithy sentence, '*Deyam dīna janāya ca vittam*' — meaning you shall give off your wealth to the poor people. But if you examine the previous line of this sloka, we find the words "*Neyam sajana saṅge cittam*", that one must also guide one's thoughts towards truth and righteousness, by leading his life in the company of good people. The Acharya does not separate the two; if the latter (namely goodness) is not there and only the former (that is charity) is present, then it is not true religion.

You would have noticed that I have never talked, specifically, of this religion or that religion; but only of religion per se. This is because these truths form the bedrock of all religions. In this connection, I am reminded of the line '*Sarvadevanamaskārāḥ kesavāṁ pratigacchati*' — that is to say, to whichever deity you offer your worship, it always goes to Kesava. In this

saying, Kesava does not mean the Hindu Lord Vishnu — it stands, in fact, for the Universal Lord, the being that is in you, in me, and in everything, and whose guiding force runs the wheel of Nature — "yena bhr̄amyate brahmacakram".

4 The Supreme Being

It is this aspect of the Supreme, or the Absolute, that I wish to discuss for the major part of this talk — for it is here that Science, Religion, and Philosophy all agree to talk the same language. In fact, I shall quote from each of these fields to show how great thinkers, the world over, have thought alike when it came to the discussion of the Essence behind the nature of all things and beings — namely the Ultimate Reality.

(i) Commenting on the ideas of Aristotle, in his book Metaphysics, Will Durant says:

"God does not create, but he moves, the world; and he moves it not as a mechanical force but as the total motive of all operations in the world; "God moves the world as the beloved object moves the lover". He is the final cause of nature, the drive and purpose of things, the form of the world; the principal of its life, the sum of its growth, the energizing entelechy of the whole. He is pure energy; the Scholastic Actus Purus — activity per se; perhaps the mystic "Force" of modern physics".

(ii) Isa Upanishad says as follows (Translation by Louis Renou):

By the Lord enveloped must this all be —
Whatever moving there is in the moving world.
Unmoving that ONE is swifter than the mind.
The sense-powers reach It not, speeding on before
Past others running. This goes standing.
In It Mātarisvan places action.

It moves; It moves not.
It is far and It is near.
It is within all this;
And it is outside of all this.

(iii) The Spanish Philosopher Spinoza of 17th century has written;

"I hold that God is the immanent, and not the extraneous, cause of all things. I say, All is in God; all lives and moves in God. And this I maintain with the Apostle Paul, and perhaps with every one of the philosophers of antiquity, although in a way other than theirs. I might even venture to say that my view is the same as that entertained by Hebrews of old".

Again he has said

"Neither intellect nor will pertains to the nature of God. The mind of God is all the mentality that is scattered over space and time, the diffused consciousness that animates the world".

(iv) Compare these with the sloka in Kena upanishad:

*"Yo manasā na manute, yenāhurmanute manah
Tadeva Brahma tvam viddhi na etad iha upasate"*

which means —

That which mind cannot conceive,
But by which mind is made to think;
Know you, that is the true Brahman,
Not this that you worship here.

(v) St. Augustine in his Sermons says exactly the same;

"This then is not God, if thou hast comprehended it;
but if this be God, thou hast not comprehended it.

This concept of the Supreme One, as being both that which constitutes everything and also that which stands outside all these, and makes them run, is the greatest contribution of Hindu Philosophy. The impact that this concept has made on the minds of scholars elsewhere is particularly evident from what the great German philosopher, Schopenhauer, has said about this mystic picture of the Supreme Being:

"The Hindus were deeper than the thinkers of Europe,
because their interpretation of the world was internal
and intuitive, not external and intellectual; the
intellect divides everything, intuition unites everything;
the Hindus saw that the "I" is a delusion;
that the individual is merely phenomena, and that
the only reality is the Infinite One — "That art thou".

(Tat tvam asi)

However, this concept has not been there only in India. It has been discovered by every great thinker, wherever he lived; in fact, many theses of Aristotle are seen to coincide with the philosophical thoughts of Ancient India. One example is the quotation from Aristotle's Metaphysics mentioned above. In fact, this concept of the Supreme Being, with emphasis on "Being" is seen even in the inscriptions of Mohenjodaro (3000 BC), where the name of God is given as "Iruvan" which means "The One who exists" in Tamil. (Source, Radhakrishnan, "The Recovery of Faith").

5. Scientist's view of the Ultimate Limits of Knowledge

The above picture is not at all inconsistent with science. As I

said earlier, science permeates every aspect of human life. I do not mean this only in the mundane sense — that we utilise the fruits of scientific enquiry whenever we do anything, such as going in a bus, or talking on the phone, or putting on the electric light in our houses. It is to be taken in a more philosophical sense, namely that Science (whose essence is the pursuit of knowledge, and the seeking out of truth) is there in whatever we do in an intelligent way. For example, a young child looks around and finds that if he goes in the direction of a wall, he hits his head against it. He finds this happening again and again, and learns from this that the wall is impenetrable; he has thus gained one unit of knowledge. All the time that man grows from his childhood, he learns things in this way, namely from experience. In fact, in children, the pleasure of learning is always there and it is bubbling. It is unfortunate that our present systems of teaching, that are adopted in our schools, often disperse these bubbles of enthusiasm, in the engulfing stream of factual information that is hurled at the young student. The students should be taught to explore Nature, be it mathematics, physics or biology, and they should be encouraged to learn by themselves, under the guidance of the teacher. Is there any hope that this will be realized?

Leaving aside this matter, it is true that even adults often introspect and try to learn about things around, but their questions are more difficult to answer. Why is everything as it is? Who am I? Where did I come from? Where will I go after my death? Is this world running by itself, or by some unseen force? In fact, the seeking of such laws governing the "Universe Around Us", is as much part of Science, as what is more commonly taken to be

its domain. Science is ever-interesting, ever-exhilarating, and ever-enjoyable. In fact, if the true spirit of science is shown in the teaching of science, namely that of presenting the facts that are available, analysing them, examining them, and taking them to bits and finding the relationship between these and then synthesising all the information thus obtained in the form of a small number of simple laws, then the spirit of science will be infused into the younger generation. I hope that, in the years to come, this will happen and that acquisition of knowledge (which is science) whether it be in the subject of mathematics, physics, biology, sociology, or even politics, is made into a scientific examination of cause and effect. I shall not elaborate on this aspect further, for lack of time.

What I shall consider in the next few minutes is to talk about the frontiers of knowledge, and as the question whether all possible knowledge will be exhaustively acquired by us, provided we have sufficient time to do so. I am afraid, the answer is — the search and this exploration of the boundaries of knowledge is not like the exploration of an island, or a forest. We know that the island, or a forest, exists over a certain area, and when that area is exhausted, it becomes known to us in full detail. Unfortunately, this can never be so in science, for the frontiers of knowledge are ever-receding; the nearer we go to the outer limits, the farther they recede. The more that we find out, the more we know about Nature, the greater does the range of the undiscovered become.

The best way of demonstrating this aspect of the frontiers of knowledge,

is to tell you some things of the information explosion during the last few decades. In every age, the scientists of that era thought that they had got at the ultimate truth; that they had really obtained the fundamental laws governing science; and that it was only a matter of finding out the details to fill up all the gaps. Such a smug attitude towards science was particularly present during the end of the last century in the field of physics. Enormous developments were made in that century, and it was thought that all the Laws of Physics were known. However, as we know now, in the beginning of this century, scientists, like Planck and Einstein, showed that even the foundations of the earlier theories were unsound, and that they had to be relaid in order to understand Nature in its naked truth. We saw the emergence of molecules and atoms; of electrons, protons, and photons. And once again, by the end of the 1920's, when relativity and quantum mechanics were fully known, it was thought that we had again reached some sort of a end. But it was not to be. During the 50's and thereafter, not only in physics, but in chemistry, and biology, there have been a tremendous expansion — not only of factual information, but even in the comprehension of these and the nature of the laws that governs these.

The explosion in Molecular Biology during the last 10 years is even more startling. We even produced new forms of life. The irrelegious may ask, 'Are we replacing God thereby?' But the scientist will answer that it is not at all the case, but that it is the same Laws of Nature that were known earlier that have been utilised for obtaining these new mysterious possibilities. We do not know where these will lead, to and what lies ahead,

6. Unending Ocean of Knowledge

I am saying all this to emphasise the fact that there will be no end to the seeking of knowledge. The scientist pictures "Nature" which he studies as consisting of the sum total of all existence, and of all the laws that govern the things that exist. One is thus irrevocably led to the ancient Hindu concept of Brahman the Supreme Entity that encompasses everything, as the equivalent of this in religion. The short, but sweeping, statements of the Katha upanishad :

'*Anoraniyan mahato mahiyan'* and '*Anadyanta*'

which may be stated as

'Atomer than the atom, mightier than the largest' and

'Having neither beginning nor end'.

really convey this concept most concretely. We must think of Nature as being infinite in space, infinitesmally divisible without end, and existing for all time. The stanza two steps earlier contains an even more comprehensive description. (This is included also in the Bhagavad Gita):

Na jāyate mriyate vā vipascin-

Nāyam kutascinna babhuva kaścit

Ajo nityah sasvato�am purano

Na hanyate hanyamāne sarire.

"THIS "intelligence" was not born and shall never die; he did not originate from anything, nor did anything other than it ever be formed. It is unborn, eternal, unchanged and standard. It is not gone when the

body dies and decays".

6. Science versus Religion:

This is the time to raise the question as to whether any part of science is opposed to the tenets of religion. In his book "Discovery of Faith", Radhakrishnan says "Religion, as it is generally understood, is opposed to the spirit of science. The method of science is empirical, while that of religion is dogmatic. Science does not rely on authority but appeals to communicable evidence that any trained mind can evaluate. Science does not admit any barriers to freedom of thought and inquiry. It welcomes new knowledge and new experience. A true scientist does not take refuge in dogmatism. His outlook is marked by modesty, self-criticism and readiness to learn from others. If we esteem freedom of inquiry, we find that it is incompatible with authoritarianism, which is the dominant feature of religion."

I dare to suggest that the above comments are not quite correct and that Radhakrishnan has taken a rather dogmatic view of religion itself, in saying that it is authoritarian, that it has dogmas, and that it is opposed to freedom of thought. However, as we have seen earlier, a truly religious person will not be opposed to freedom of thought, since for him the source of thought itself is God. If belief in the concept of God as being the guiding spirit behind the workings of Nature is accepted, then the fundamental basis of Science and that of Religion become one and the same. Both believe in Law, Truth, and Order. They differ only in that one says that it is derived from the Supreme Being, while the other says

that it is the property of Nature, without asking further the question as to why this property exists?

So, we see that, instead of looking for the scientific basis of religion, which we started to examine, we have come to the conclusion that true religious inquiry encompasses within itself the whole of Science. Advaita, or ONENESS of the power behind Existence, is the essence of both; but this ONE exhibits itself in a million things and a million ways. We have to study all these in the true scientific spirit, and ascend upwards, seeking more and more Universal Laws that encompass the whole range of Knowledge. Ultimately one transcends even the bounds of knowledge and thought, and realizes that Spirit which is within all of Existence, and which at the same time encompasses it all — an entity that is beyond comprehension of our limited mind.

So, I end with some hymns describing that Supreme Spirit:

"Aham Brahmasmi, Brahm evaham asmi, Brahmaeva Satyam"

(I am Brahman; I am nothing but Brahman; Brahman is all Truth)

— Hindu prayer

"Ana al-Haqq" (I am Truth) — Al Hallāj (Sufi)

"Satyameva jayate" (Only truth shall prevail) — Buddha

"Truth is God" — Gandhi

I would add to these the following from my creed as examples of the manifestations of the Lord;

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(Summary of Presidential Address to the Physics Section of the National Academy of Sciences, India, Allahabad, held in Cochin).

Introduction

Fourier transforms have found wide application in almost all branches of physics — in particular in communication theory, optics, x-ray crystallography and quantum mechanics. There is an extensive literature in the field connected with its basic theory. There are also excellent books like that of Ron Bracewell (1) which deal with the basic theory with reference to applications essentially in Communication Theory; similarly, applications in optics and crystallography are treated in specialized books e.g. those of Goodman (2) and Ramachandran (3). However, an overall treatment of Fourier transforms in general, looked at both from the point of view of the pure mathematician and from the point of view of the physicist, or the engineer, who applies it, is not readily available. In this lecture, we shall consider such aspects of Fourier transforms which are fundamental in nature, but which at the same time are intimately connected with practical applications. The new results, which we will discuss, appear to have very extensive validity for the Fourier transforms of all "Physical Functions".

* The studies reported here were carried out in collaboration with

Dr. S.H. Kulkarni.

It is an interesting fact that the Fourier transform always exists for a physical function. A physical function may be defined as a function representing, for example, the density of a real object having finite dimensions and finite total mass. The two essential conditions are "absolute integrability" (AI) and "bounded support" (BS). The former one is slightly different from the idea of finite total mass; but the two agree if the density everywhere is positive, which is certainly true for mass. More generally, it is the integral of the modulus of the function that must be positive for the criterion of AI to be satisfied. This gets modified to $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx \leq K$ in quantum mechanics, for which case we replace AI by this condition of "square integrability" (SQI). It is readily shown that if BS is true, then $SQI \Rightarrow AI$.

The condition BS represents the fact that the extension of the object in space is finite. Thus, for an one-dimensional function $f(x)$, it is non-zero along the x-axis only for a finite range of x — e.g. $f(x) \neq 0$ only for $-a \leq x \leq +b$.

We shall restrict our theory to this one-dimensional example; reserving the extension to a larger number of dimensions to the end. Thus if $f(x)$ is both AI and BS, then the following results can be proved for its Fourier transform $F(X)$, defined by

$$F(X) = \int_{-\infty}^{+\infty} f(x) \exp 2\pi i X x dx \quad (1)$$

1. The Fourier transform exists right from $-\infty$ to $+\infty$ for X , or

$$F(X) \text{ has unbounded support (UBS)} \quad (2)$$

2. $F(X)$ is also infinitely differentiable (ID) for this whole range of X . The condition for ID will be shown to be represented by the condition (5) below :

$$\left| \frac{d^j F(\lambda)}{d\lambda} \right| \leq KC^j \quad (3)$$

3. $F(X)$ is, in addition, infinitely oscillatory (IO). One of the conditions for IO is that

$$\left| F(X) \right|^2 = 0 \text{ an infinite number of times for } \left. \begin{array}{c} \\ \\ -\infty < \lambda < +\infty \end{array} \right\} \quad (4a)$$

More generally $d\left| F(X) \right|^2/dX = 0$ an infinite number of times, so that

$$\left. \begin{array}{c} \text{The intensity } \left| F(X) \right|^2 \text{ has an infinite number} \\ \text{of maxima and minima} \end{array} \right\} \quad (4b)$$

Still more generally,

$$\left. \begin{array}{c} d^m \left| F(X) \right|^2 / dX^m = 0, \text{ an infinite number of times for} \\ \text{some finite } m \end{array} \right\} \quad (4c)$$

Thus, either the modulus-square of the function, or some derivative of it, goes through maxima and minima an infinite number of times. Actually, (4a) is very common, and the function itself vanishes at regular intervals and there are ripples in the intensity of the Fourier transform, or diffraction pattern, which do not completely vanish, (although they may die away in magnitude) with increasing values of $|X|$. Some of these will be proved in a brief detail in the lecture.

Coming to practical applications, the most interesting one is the

result (1) — namely that the Fourier transform of a function of BS (which is also AI) has UBS. Thus, if a particle, in a quantum mechanical system, is confined within a box, then its momentum (whose eigenfunction $\phi(p)$ is the Fourier transform of its wave function $\psi(x)$), exists for all values of p from $-\infty$ to $+\infty$. In other words, there is no upper limit to the value of the momentum of a particle confined to a box from $x = -a$ to $x = a$. This is possibly the explanation of the tunnelling effect observed in such systems, which happens because the momentum, and consequently the energy, can take up large enough values, so that the particle can go over an energy barrier, to regions outside the box. Thus, we have a simple general, physically understandable, explanation of why tunnelling is a universal phenomenon in quantum mechanical systems.

Considering the result I0 (given by (4)), which always goes along with result (3), namely ID, it means that the diffraction pattern of a finite object always exhibits an infinite number of ripples; or an infinite number of oscillatory variations occur in its intensity. Neglecting the case (4c) which is rather specialized, we may say that the function $|F(X)|^2$ either has an infinite number of zeros, or has an infinite number of oscillations. What is more interesting is the fact that the period of these oscillations remains steady for sufficiently large X , and this period corresponds to the range of the BS, namely $2a$, if $f(x)$ is non-zero only for values of x from $-a$ to $+a$. Thus, for large X the diffraction pattern is dominated by the distance between the two outer limits on the left and right hand side, within which the function exists.

This is very interesting fact which has several applications in

optical diffraction. We shall only mention one. Consider a two-dimensional object — say a plane aperture of arbitrary shape. Then its diffraction pattern along the direction X is determined completely by the projection, of the function representing the amplitude of the light wave within the aperture, on x-axis. Suppose this function exists from -a to + b (say). Then, the limiting period of the diffraction pattern for large X is dominated by that corresponding to the distance $\ell = (a+b)$, which is the magnitude of the BS along the x-axis. This result does not seem to be generally recognized, although the lecturer remembers that Prof. Sir C.V. Raman always stated it and would derive it from semi-intuitive arguments, as long ago as the early 1940's. In fact, the IO nature of the F.T. of a function of BS has also applications in "Image Reconstruction". It can be shown from our theory, quite generally, that if the F.T. of a finite object of BS (which is of UBS) is truncated and the object reconstructed from the truncated F.T., then the reconstruction can never be perfect, whatever corrections be applied, although they may serve to reduce the errors.

The above would indicate that there are many interesting possibilities regarding Fourier transforms, of practical utility, which can be derived from our new results as given in Eqns. (2), (3) and (4).

References

1. Bracewell, R. "The Fourier Transform and Its Applications", 2nd Edn, McGraw-Hill, New York, 1978.
2. Goodman, J.W. "Introduction to Fourier Optics", McGraw-Hill, New York, 1968.
3. Ramachandran, G.N. "Fourier Methods in Crystallography", Wiley-Interscience, New York, 1970.

Studies on
M A T R I X A L G E B R A F O R L O G I C
A N D
F O U R I E R T R A N S F O R M S O F P H Y S I C A L . F U N C T I O N S

(Brief summary of work done in the Mathematical
Philosophy Group in 1979-81)

Presented to Prof. Satish Dhawan as a
memento on his retirement from the Institute

G.N. Ramachandran
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MATPHIL Reports No.22, July 1981.

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July 1981.

P A R T I

MATRIX METHODS FOR SENTENTIAL LOGIC

General Theory — G.N. Ramachandran

Fortran Programs — T.A. Thararaj

Electronic analog computer — R.E.C.Johnson

Pascal Program — I.A.Abdii.

1. Introduction

In our department, we have been working out novel techniques for analysing and solving logical equations that occur in any theorem — for that matter, in any set of statements whatsoever forming a connected argument. It is well known that logic bears the same relation to thought, as grammar bears to language. Essentially, logic only verifies that the different statements are consistent with one another, and does not care whether they are meaningful or not. (As regards this, there is a difference of opinion between Classical Indian logicians and western logicians, for in India, it was believed that logic is of no purpose, unless it is used in connection with statements that have a proper semantic content also associated with them. We shall not discuss this further).

In modern logic, as has been developed during the last century, it has been realised that it can be divided into two aspects — namely, a) Sentential Logic, in which only unquantified statements are made such as good, bad, is present etc., and b) Quantified Predicate Logic, in which we emphasize on the fact whether the statement is true for all cases or for some cases or for no case etc., In other words, a quantifier which shall consist of two types (For all (\forall) and there exists (\exists)) are employed.

The Theory of Sentential Logic is supposed to be complete and well understood. However there a program, or algorithm, for working every argument in Sentential logic does not appear to be available and the development of such algorithms is the purpose of our investigations.

2. New Features of our Calculus for Sentential Logic

In doing this, we have come across some novel features, which are, however, really part and parcel of Sentential Logic — namely in that they necessarily follow from the accepted formalism. Thus, if one checks a statement like "a and b is false" given that "a is false", and ask the question, "Is b true or false?", then the answer is "b may be true or false". This type of "doubtful" result arises often, whenever the so called reverse operator is applied. (In this particular case, it is reverse A, or $\leftarrow A$). In the same way, if "a and b is true" and "a is false", and we enquire "What is b? ", it will turn out that "b is neither true nor false", leading to what may be called the "impossible" state of b.

Thus, in general, we find that four logical states have to be postulated — namely T = true, F = false, D = doubtful and X = impossible, instead of only two — namely T and F — as used in classical logic. The existence of "doubt" in epistemology, and its removal being the essence of acquiring knowledge, was the principal thesis of the Jaina philosophers of Ancient India, who gave this the name "Syādvāda" (theory of "may be"). Hence, we have named our development of Sentential Calculus as the Syād-Nyāya-System (SNS in short; Nyāya = logic). As mentioned above, SNS has two new innovations — a) the specification of reverse operators and b) the introduction of the doubtful and impossible states that are brought in thereby.

There is one more new type of operator that becomes necessary when the above two innovations are applied. This occurs when information about the truth value of a term comes from two different sources. For combining these, we need a new operator, which we have named "with" (W), in addition to the classical operator "and" (A) and "or" (O), as binary operators. Thus,

$$\begin{aligned}
 \underline{T} \swarrow \underline{W} \searrow \underline{F} &= \underline{X} \\
 \underline{T} \swarrow \underline{W} \searrow \underline{T} &= \underline{T} \\
 \underline{T} \swarrow \underline{W} \searrow \underline{F} &= \underline{F} \quad (1) \\
 \underline{T} \swarrow \underline{W} \searrow \underline{D} &= \underline{T} \\
 \underline{F} \swarrow \underline{W} \searrow \underline{D} &= \underline{F}
 \end{aligned}$$

This newly introduced operator \swarrow is not at all new, because it is invariably used in proving mathematical theorems. Thus, a theorem may not known to be true or false (in \underline{D} state) and a new proof gives that it is true (\underline{T} state). Then it can be said that it is true (\underline{T} prevails over \underline{D}). On the other hand, if we prove that something is \underline{T} , and \underline{F} , by two methods, both of which are valid, then the resultant state is $\underline{T} \swarrow \underline{W} \underline{F} = \underline{X}$, or impossible and obviously the starting point of one or the other method must be wrong. (This is the essence of the reductio ad absurdum method of proof).

3. Practical applications

In applying the above, we found out various techniques of utilizing the new formalism. There is no time to discuss these in detail; but the nature and the format of this will be evident from the examples given below. We find that every logical argument can be represented by a logical graph. (For an example of a logical graph, see the report of Abdi at the end of this part.) In fact, if one just takes some terms and make logical connections between them according to any permissible graph (decided by a few simple rules), then it will correspond to a possible logical argument; it is a different matter whether this argument is valid, or invalid, and whether it contains contradictions, or undefinable data. In other words, we have a universal connection between graph theory and logical arguments. In the same way, in implementing

the above, we found that the best technique is to use Boolean matrix algebra. Thus we represent the states by means of two-element Boolean vectors as below:

$$\begin{aligned}\langle T \rangle &= (1 \quad 0) \\ \langle F \rangle &= (0 \quad 1) \\ \langle D \rangle &= (1 \quad 1) \\ \langle X \rangle &= (0 \quad 0)\end{aligned}\tag{2}$$

and connectives by 2×2 Boolean matrices — for example,

$$\begin{aligned}\langle A \rangle &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \quad \langle E \rangle = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \langle O \rangle &= \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}; \quad \langle I \rangle = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}\end{aligned}\tag{3}$$

The newly defined operator "with" has the property that

$$\underline{a} \underset{\sim}{\text{W}} \underline{b} = \underline{c} \tag{4a}$$

corresponds to

$$\underline{a}_\alpha \otimes \underline{b}_\alpha = \underline{c}_\alpha; \quad \underline{a}_\beta \otimes \underline{b}_\beta = \underline{c}_\beta \tag{4b}$$

where the operator \otimes is the Boolean multiplication operator. Thus,

$$\begin{aligned}\underline{a}_T \otimes \underline{b}_F &= (1 \quad 0) \otimes (0 \quad 1) \\ &= (1 \otimes 0 \quad 0 \otimes 1) \\ &= (0 \quad 0) = \underline{c}_X\end{aligned}\tag{5}$$

4. Example of a problem from a standard book on logic

We take the problem stated as follows in the book 'Introduction Set Theory and Logic' by Robert R. Stoll (Freeman, San Francisco and London, 1961)

$$\begin{aligned} W \vee P &\rightarrow I, \quad I \rightarrow C \vee S, \quad S \rightarrow U, \\ \neg C \wedge \neg U &\leftarrow F \neg W \end{aligned} \quad (6)$$

The problem requires that, given the four equations in the left hand side, we should prove that W is always false. For doing this in our formalism, we have written these four as four equations in our notation:

$$(W \vee p) Y = i \quad (7a)$$

$$i Y = (C \vee S) \quad (7b)$$

$$S Y = u \quad (7c)$$

$$(C N) A (u N) = T \quad (7d)$$

Using p , i , C (One possible combination of inputs), the other three (S , u , W) can be predicted using the following three equations (8a), (8b), and (8c)

$$(i V) \swarrow \swarrow p = W \quad (8a)$$

$$(i Y) \swarrow \swarrow C = S \quad (8b)$$

$$(S Y) \swarrow \swarrow ((T A (C N)) N) = u \quad (8c)$$

We shall not go into the details except to mention that the full formalism of our technique has been written as a FORTRAN program called MATLOG which can be run on DEC-10, and which can solve any general problem in Sentential logic, provided the graph of the set of equations is given (There is, of course, the problem of converting the set of equations to be in a suitable order, so

that they are implementable (by which we mean that a later equation always uses only those inputs that are either original inputs, or those obtained from the previous inputs). This problem is being examined in great detail by Abdi).

The print out of MATLOG is given in pages 14-24. The Fortran equations corresponding to the present problem (Eqs. 8a, b, c) are given in page 8 and output for \underline{p} , \underline{i} , \underline{c} , \underline{s} , \underline{u} , \underline{w} in tabular form is given in page 9.

On examining the table, it will be seen that, for the first seven possible inputs, there is contradiction somewhere among \underline{s} , \underline{u} , \underline{w} while the last one has no contradictions and this is the only set of inputs permissible for \underline{p} , \underline{i} , \underline{c} namely \underline{F} , \underline{F} , \underline{F} . For this set of inputs, \underline{w} is also \underline{F} . In fact, we show, in this way, that the only set of permissible inputs for the equations given by Stoll demands W is always False. However, it also demands that \underline{p} , \underline{i} , \underline{c} are also false, and only \underline{u} is capable of having either the \underline{T} or the \underline{F} state. In other words, we have proved five times as much as what is given by Stoll using only three steps, involving three equations, while he uses as many as thirteen steps to prove the one result, namely $\underline{w} = \underline{F}$. Thus it appears that, this matrix method, or technique, has great potentialities for applications for analysing sentences in the so-called propositional logic.

..... contd.(8)

PROGRAM FOR THE PROBLEM TAKEN FROM STOLL'S BOOK

```

DIMENSION MVP(2),MVI(2),MVC(2)
DATA MVP,MVI,MVC/'T','F','T','F','T','F'/
WRITE (3,4)
FORMAT (20(/) 8X,'TRUTH TABLE FOR THE PROBLEM')
C' TAKEN FROM STOLL''S BOOK'//23X,'P',3X,'I',3X,'C',5X,'S',
C3X,'U',3X,'W')
DO 2 I=1,2
DO 2 J=1,2
DO 2 K=1,2
MUV = MBRN(MUNN(MVI(J),MZVE),MZOE,MVP(I))
MVS = MBRN(MUNN(MVI(J),MZYE),MZOE,MVC(K))
MVU = MBSN(MUNN(MVS,MZYE),MSWW,MON(MBRN(MSTR,MZAE,MON(MVC(
K))))))
WRITE (3,3)MVP(I),MVI(J),MVC(K),MVS,MVU,MUV
FORMAT (/20X,3(3X,A1),2X,3(3X,A1))
CONTINUE
STOP
END

```

TRUTH TABLE FOR THE PROBLEM TAKEN FROM STOLL'S BOOK

P	I	C	S	U	W
T	T	T	D	X	D
T	T	F	T	X	D
T	F	T	D	X	X
T	F	F	D	F	X
F	T	T	D	X	D
F	T	F	T	X	D
F	F	T	D	X	F
F	F	F	D	F	F

5. Logic Program for the Pocket Calculator TI-59.

The principles of SNS logic have also been programmed for a programmable pocket calculator — namely TI-59. This program is different from MATLOG and is based on an earlier version NYAYA2 prepared for Dec10. The main program takes only 384 steps, and since this calculator has plenty of spare memory, many problems of practical interest can be worked out using this, although this calculator takes a much longer time. The program — TINY1 is illustrated in pages 25 to 29. The sub-program for the special problem, namely the one from Stoll's book, written for TI59, is given in page 11, which also contains the output for the eight possible input state combinations mentioned earlier. In this calculator T, E, D, X are coded as 1.0, 0.1, 1.1 and 0.0 respectively. It indicates the impossible state X whenever it occurs by printing a question mark (?) opposite the output. In this way, it will be seen that only the last set of data are free of question marks exactly as we have already indicated.

6. Electronic analog computer

Actually, all the programs mentioned earlier — in particular NYAYA1 and NYAYA2 — were the outcome of the attempts to represent logical equations in an analog computer using logic chips. The only logic chips that have been used are those for AND, OR, XOR, and NOT (inverters). Using these in various combinations, SNS logic has been represented in our analog machine, which has been given the name ESNY (Electronic Syad-Nyaya Yantra). In this, the two Boolean elements a_{α} , a_{β} , of a term a , are represented by the two states 1 and 0 corresponding to existence and non-existence of voltage in the two lines α and β . The matrices, or their logical equivalents, are very simply represented by a combination of logic chips. The details are not given here since a long report (Matphil Report No. 13) is available on this. The

TINYI program for the problem taken from STULL's book

Subprogram

Results

states of a term are represented on the panel by green lights for \underline{T} , red lights for \underline{F} , and both green and red glowing for the \underline{D} state. When the \underline{X} state occurs, neither green nor red light glows; but a yellow flashing light occurs, along with an alarm in the form of a siren. Hence the occurrence of an impossible state is immediately indicated by the siren sounding, and the cause of this can be investigated.

The construction of the various connectives, both normal and reverse, and also the new connectives like \underline{W} (with) can be implemented very readily using only the very small number of elementary electronic components mentioned above.

The example of Stoll's problem will be demonstrated, and it will be noticed that, for all the first seven inputs of Table 1, one of the outputs at least is \underline{X} as indicated by the siren sounding. The siren is absent only for the last case ($\underline{p} = \underline{F}$, $\underline{i} = \underline{F}$, $\underline{c} = \underline{F}$), which gives $\underline{s} = \underline{D}$, $\underline{u} = \underline{F}$, $\underline{w} = \underline{F}$, exactly as given by the FORTRAN program and TINY pocket calculator program.

The three types of calculations — either using the DEC10, or TI59, or ESNY — are of different capabilities, the last two of which can be used on line in the laboratory and could be readily changed whenever we want to study a new problem, or a variation of a problem, have been very useful. We are now investigating the special possibilities that come out of "contradiction" and "doubt". The analysis of a logical graph in such cases is not straightforward, and some more tests have to be made. For this purpose, a readily interacting computer is much more valuable than a powerful computer.

7. Conclusion

We have recently started to work on Quantifier Logic and we believe that the same matrix method, with careful generalizations,

can be applied for Quantifier Logic. In this case, a term (α) has two Boolean elements (a_α , a_β) to represent the SNS state of T , F , D or X and three Boolean elements (a_γ , a_ζ , a_ϵ), in general, to represent the quantified states, which in general are eight in number. A single additional Boolean element (a_ζ) is sufficient, if we want to represent only the two states \forall and \exists . This field is being explored further.

Listing of MATLOG program

1. (a) Listing of the file LIST.FOR.

C.....PROGRAM LIST.FOR.

```
DIMENSION MATDAT(16,5)
COMMON/MATD/MATDAT
DATA MATDAT/'MZEE','MZEM','MZAЕ','MZAM','MZYM','MZYЕ',
C'MZVM','MZVE','MZOM','MZOЕ','MZRE','MZRM','MZCE','MZCM',
C'MZDE','MZDM',1,0,1,0,0,1,0,1,0,1,1,0,1,0,0,1,0,1,1,0,
CO,1,0,1,1,0,0,1,1,0,0,1,0,1,0,1,1,0,0,1,0,1,1,0,1,0,1,0,
C1,0,0,1,0,1,0,1,1,0,0,1,0,1,1,0,0,1,0,1,1,0/
DATA,MZEE,MZEM,MZAЕ,MZAM,MZYM,MZYЕ,MZVM,MZVE,MZOM,MZOЕ,
CMZRE,MZRM,MZCE,MZCM,MZDE,MZDM/'MZEE','MZEM','MZAЕ','MZAM',
C'MZYM','MZYЕ','MZVM','MZVE','MZOM','MZOЕ','MZRE','MZRM',
C'MZCE','MZCM','MZDE','MZDM'/
DATA MSTR,MSFL,MSDF,MSXX/'T','F','D','X'/
COMMON /MS/MSTR,MSFL,MSDF,MSXX
DATA MSMM,MSWW,MSUU,MSGG/'M','W','U','G'/
```

1. (b) Listing of MATLOG programs.PROGRAM MATLOGI Functions for Vector and matrix components.

1.

FUNCTION MA(MVA)

C THIS SUBPROGRAM COMPUTES THE ALPHA COMPONENT OF THE VARIABLE MVA.

COMMON /MS/ MSTR,MSFL,MSDF,MSXX

MA = 0

IF ((MVA .EQ. MSTR) .OR. (MVA .EQ. MSDF)) MA = 1

END

2.

FUNCTION MB(MVA)

C THIS SUBPROGRAM COMPUTES THE BETA COMPONENT OF THE VARIABLE MVA

COMMON /MS/ MSTR,MSFL,MSDF,MSXX

MB = 0

IF ((MVA .EQ. MSFL) .OR. (MVA .EQ. MSDF)) MB = 1

END

3.

FUNCTION MSTATE(MAA,MBB)

C THIS SUBPROGRAM COMPUTES THE MATLOG STATE OF THE VARIABLE MVA

C GIVEN ITS COMPONENTS

COMMON /MS/ MSTR,MSFL,MSDF,MSXX.

IF (MAA .EQ. 1) GO TO 1

IF (MBB .EQ. 1) GO TO 2

MSTATE = MSXX;RETURN

2 MSTATE = MSFL;RETURN

1 IF (MBB .EQ. 1) GO TO 3

MSTATE = MSTR;RETURN

3 MSTATE = MSDF

END

4.

FUNCTION KK1(MZKL)

C THIS SUBPROGRAM FINDS THE ALPHA-ALPHA COMPONENT OF THE MATRIX

C GIVEN BY THE MATRIX NAME OF MZKL.
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I=1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK1 = MATDAT(I,2);RETURN
2 CONTINUE
END

5. FUNCTION KK2(MZKL)

C THIS SUBPROGRAM FINDS THE ALPHA-BETA COMPONENT OF THE MATRIX
C GIVEN BY THE MATRIX NAME OF MZKL.
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK2 = MATDAT(I,3);RETURN
2 CONTINUE
END

6. FUNCTION KK3(MZKL)

C THIS SUBPROGRAM FINDS THE BETA-ALPHA COMPONENT OF THE MATRIX
C GIVEN BY THE MATRIX NAME OF MZKL.
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK3 = MATDAT(I,4);RETURN
2 CONTINUE
END

7. FUNCTION KK4(MZKL)

C THIS FUNCTION FINDS THE BETA-BETA COMPONENT OF THE MATRIX
C GIVEN BY THE MATRIX NAME MZKL.

```
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (MZKL .NE. MATDAT(I,1)) GO TO 2
KK4 = MATDAT(I,5);RETURN
2 CONTINUE
END

8. FUNCTION MAT(K1,K2,K3,K4)
C THIS SUBPROGRAM COMPUTES THE MATRIX NAME GIVEN ITS ELEMENTS
DIMENSION MATDAT(16,5)
COMMON /MATD/MATDAT
DO 2 I = 1,16
IF (K1 .NE. MATDAT(I,2)) GO TO 2
IF (K2 .NE. MATDAT(I,3)) GO TO 2
IF (K3 .NE. MATDAT(I,4)) GO TO 2
IF (K4 .NE. MATDAT(I,5)) GO TO 2
MAT = MATDAT(I,1);RETURN
2 CONTINUE
END
```

II Functions for Vector-matrix operations.

```
9. INTEGER FUNCTION BOOLAN(IX)
C THIS SUBPROGRAM FINDS THE BOOLAN EQUIVALENT OF THE INTEGER
C NUMBER IX.
BOOLAN = 1
IF (IX .EQ. 0) BOOLAN = 0
RETURN
END

10. INTEGER FUNCTION COMPN(N)
C THIS SUBPROGRAM PERFORMS THE COMPLEMENTATION OPERATION
C ON THE NUMBER N
```

```
      COMPN = 1-N
      END

11. INTEGER FUNCTION COMPV(MVA)
C   THIS SUBPROGRAM PERFORMS THE COMPLEMENTATION OPERATION
C   ON THE VARIABLE MVA
      COMMON/MS/MSTR,MSFL,MSDF,MSXX
      COMPV = MSTATE(1-MA(MVA),1-MB(MVA))
      END

12. INTEGER FUNCTION COMP(MZKL)
C   THIS SUBPROGRAM PERFORMS THE COMPLEMENTATION OPERATION ON
C   THE MATRIX MZKL.
      L1 = 1-KK1(MZKL)
      L2 = 1-KK2(MZKL)
      L3 = 1-KK3(MZKL)
      L4 = 1-KK4(MZKL)
      COMP = MAT(L1,L2,L3,L4)
      END

13. INTEGER FUNCTION TRAN(MZKL)
C   THIS SUBPROGRAM PERFORMS THE TRANSPOSE OPERATION ON THE
C   MATRIX MZKL.
      TRAN = MAT(KK1(MZKL),KK3(MZKL),KK2(MZKL),KK4(MZKL))
      END

14. INTEGER FUNCTION TRCP(MZKL)
C   THIS SUBPROGRAM PERFORMS THE TRANSPOSE-COMPLEMENT OPERATION
C   ON MZKL.
      INTEGER TRAN,COMP
      TRCP = TRAN(COMP(MZKL))
      END

15. FUNCTION T(MVA)
C   THIS SUBPROGRAM COMPUTES THE TRUTH VALUE OF THE VECTOR MVA.
```

```

COMMON /MS/MSTR,MSFL,MSDF,MSXX
SQ = MA(MVA)*MA(MVA)+MB(MVA)*MB(MVA)
IF (SQ .EQ. 0.0) GO TO 3
T = (MA(MVA)*MA(MVA))/SQ
RETURN
3 T = 8.0
END

16. INTEGER FUNCTION VEC(TMVA)
C THIS FUNCTION FINDS THE VECTOR MVA, GIVEN ITS TRUTH VALUE TMVA.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
IF (TMVA .EQ. 8.0) GO TO 3
T1 = TMVA; T2 = 1-TMVA
T = (T1*T1+T2*T2)
TA = T1/T; TB = T2/T
VEC = MSTATE ( INT(TA + 0.001),INT(TB + 0.001))
RETURN
3 VEC = MSXX
END

17. INTEGER FUNCTION BOLVVP(MVA,MVB)
C THIS SUBPROGRAM PERFORMS THE BOOLEAN VECTOR-VECTOR PRODUCT
C OF THE VECTORS MVA AND MVB.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
INTEGER BOOLAN
BOLVVP = BOOLAN(MA(MVA)*MA(MVB)+MB(MVA)*MB(MVB))
END

18. INTEGER FUNCTION BOLVMP(MVA,MZKL)
C THIS SUBPROGRAM PERFORMS THE OPERATION BOOLEAN VECTOR-MATRIX
C PRODUCT OF THE MATRIX MZKL AND THE INPUT VECTOR MVA.
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
INTEGER BOOLAN
MAMVB = BOOLAN(MA(MVA)*KK1(MZKL)+MB(MVA)*KK3(MZKL))

```

```
MBMVB = BOOLAN(MA(MVA)*KK2(MZKL)+MB(MVA)*KK4(MZKL))
BOLVMP = MSTATE(MAMVB,MBMVB)
END
```

19. INTEGER FUNCTION BOLMVP(MZKL,MVA)
C THIS SUBPROGRAM PERFORMS THE BOOLEAN MATRIX VECTOR PRODUCT
C OF THE MATRIX MZKL ON THE VECTOR MVA.

```
COMMON /MS/MSTR,MSFL,MSDF,MSXX
INTEGER BOOLAN
MAMVB = BOOLAN(KK1(MZKL)*MA(MVA) + KK2(MZKL)*MB(MVA))
MBMVB = BOOLAN(KK3(MZKL)*MA(MVA) + KK4(MZKL)*MB(MVA))
BOLMVP = MSTATE(MAMVB,MBMVB)
END
```

20. INTEGER FUNCTION BOLMMP(MZKL,MZKM)
C THIS SUBPROGRAM PERFORMS THE BOOLEAN MATRIX-MATRIX
C PRODUCT.

```
INTEGER BOOLAN
K1 = BOOLAN(KK1(MZKL)*KK1(MZKM)+KK2(MZKL)*KK3(MZKM))
K2 = BOOLAN(KK1(MZKL)*KK2(MZKM)+KK2(MZKL)*KK4(MZKM))
K3 = BOOLAN(KK3(MZKL)*KK1(MZKM)+KK4(MZKL)*KK3(MZKM))
K4 = BOOLAN(KK3(MZKL)*KK2(MZKM)+KK4(MZKL)*KK4(MZKM))
BOLMMP = MAT(K1,K2,K3,K4)
END
```

III Standard unary and binary connectives in MATLOG.

21. FUNCTION MUNN(MVA,MZKL)
C THIS SUBPROGRAM PERFORMS THE MATRIX UNARY OPERATION MZKL ON MVA.
C THIS IS THE SAME SUBPROGRAM AS BOLVMP.

```
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
INTEGER BOLVMP
MUNN = BOLVMP(MVA,MZKL)
END
```

22.

```
FUNCTION MUNT(MVA,MZKL)
C THIS FUNCTION PERFORMS THE MATRIX UNARY OPERATION OF THE
C transpose of the matrix MZKL on the input MVA.
INTEGER BOLVMP,TRAN
MUNT .. BOLVMP(MVA,TRAN(MZKL))
END
```

23.

```
FUNCTION MBDN(MVA,MZKL,MVB)
C THIS SUBPROGRAM PERFORMS THE BINARY OPERATION CORRESPONDING
C TO THE MATRIX MZKL ON THE INPUT VECTORS MVA AND MVB.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
INTEGER COMP,BOOLAN
MVG1 = MA(MVA)*KK1(MZKL)+MB(MVA)*KK3(MZKL)
MVG2 = MA(MVA)*KK2(MZKL)+MB(MVA)*KK4(MZKL)
MAMVC = BOOLAN(MVG1*MA(MVB)+MVG2*MB(MVB))
MZKL1 = COMP(MZKL)
MVG1 = MA(MVA)*KK1(MZKL1)+MB(MVA)*KK3(MZKL1)
MVG2 = MA(MVA)*KK2(MZKL1)+MB(MVA)*KK4(MZKL1)
MBMVC = BOOLAN(MVG1*MA(MVB)+MVG2*MB(MVB))
MBDN = MSTATE(MAMVC,MBMVC)
END
```

24.

```
FUNCTION MBDT(MVB,MZKL,MVA)
C THIS SUBPROGRAM PERFORMS THE MATRIX BINARY DIRECT OPERATION OF
C THE transpose of the matrix MZKL ON THE INPUTS MVB AND MVA.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
INTEGER TRAN
MBDT = MBDN(MVB,TRAN(MZKL),MVA)
END
```

25.

```
FUNCTION MBRN(MVC,MZKL,MVA)
C THIS SUBPROGRAM PERFORMS THE BINARY REVERSE OPERATION,MZKL
C ON MVC AND MVA.
```

```
COMMON /MS/MSTR,MSFL,MSDF,MSXX
INTEGER COMP,BOLVMP
IF (MVA .EQ. MSXX) GO TO 1
IF ((MVC .EQ. MSDF) .OR. (MVC .EQ. MSXX)) GO TO 2
MZRKL = MZKL
IF (MVC .EQ. MSFL) MZRKL = COMP(MZKL)
MBRN = BOLVMP(MVA,MZRKL);RETURN
2 MBRN = MVC;RETURN
1 MBRN = MSXX
END
```

26.

```
FUNCTION MBRT(MVC,MZKL,MVB)
C THIS SUBPROGRAM PERFORMS THE MATRIX BINARY REVERSE OPERATION
C OF THE TRANPOSE OF THE MATRIX MZKL ON INPUTS MVC AND MVB.
COMMON /MS/MSTR,MSF,MSDF,MSXX
INTEGER TRAN
MBRT = MBRN(MVC,TRAN(MZKL),MVB)
END
```

IV Other unary and binary functions for logical connectives.

27.

```
FUNCTION MOE(MVA)
C THIS SUBPROGRAM PERFORMS THE OPERATION EQUAL TO ON THE VECTOR
C REPRESENTED BY MVA.
COMMON /MS/MSTR,MSFL,MSDF,MSXX
MOE = MVA
END
```

28.

```
FUNCTION MON(MVA)
C THIS SUBPROGRAM PERFORMS THE OPERATION NEGATION ON THE
C VARIABLE MVA.
COMMON /MS/ MSTR,MSFL,MSDF,MSXX
MON = MSTATE(MB(MVA),MA(MVA))
END
```

29. FUNCTION MOM(MVA)

C THIS SUBPROGRAM PERFORMS THE OPERATION COMPLEMENTATION ON MVA

COMMON /MS/MSTR,MSFL,MSDF,MSXX

MOM = MSTATE(1-MA(MVA),1-MB(MVA))

END

30. FUNCTION MUSN(MVA,MSNN)

C THIS SUBPROGRAM PERFORMS THE SNS UNARY OPERATION MSNN ON

C THE INPUT MVA.

COMMON /MS/MSTR,MSFL,MSDF,MSXX

IF (MSNN .EQ. 'M') GO TO 1

RETURN

1 MUSN = MSTATE(1-MA(MVA),1-MB(MVA))

RETURN

END

31. FUNCTION MBSN(MVA,MSNN,MVB)

C THIS SUBPROGRAM PERFORMS THE SNS BINARY OPERATION MSNN

C (K MAY BE W,U,G) ON THE INPUTS MVA AND MVB.

COMMON /MS/ MSTR,MSFL,MSDF,MSXX

INTEGER BOOLAN

IF ((MVA .EQ. MSXX) .OR. (MVB .EQ. MSXX)) GO TO 11

IF (MSNN .EQ. 'W') GO TO 1

IF (MSNN .EQ. 'U') GO TO 2

IF (MSNN .EQ. 'G') GO TO 3

1 MAMVC = MA(MVA)*MA(MVB)

MBMVC = MB(MVA)*MB(MVB)

MBSN = MSTATE(MAMVC,MBMVC)

RETURN

2 MAMVC = BOOLAN(MA(MVA)+MA(MVB))

MBMVC = BOOLAN(MB(MVA)+MB(MVB))

MBSN = MSTATE (MAMVC,MBMVC)

RETURN

```
3 MBSN = MSFL
   IF (MVA .EQ. MVB) MBSN = MSTR
   RETURN
11 MBSN = MSXX
   END
```

LISTING OF TINY 1 PROGRAM

Core of the Program

Classical FC		Classical NOT		Classical AND		Classical OR	
0	0	1	0	0	0	1	1
0	1	0	1	0	1	0	1
1	0	1	0	1	0	1	1
1	1	0	0	1	1	1	1

X-priority	
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
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86	86
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89	89
90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

SUBROUTINES

SNS Analogs of Classical Operators

2
The following table gives the results of the experiments made by Mr. J. C. Goss and Mr. W. H. Dyer at the Bureau of Fisheries, Washington, D. C., on the growth of young fish under different conditions of temperature and food supply.

SNS Analogs of Classical Operators (Contd)

Binary (\mathbb{Q})

220	00000000000000000000000000000000
221	00000000000000000000000000000001
222	00000000000000000000000000000010
223	00000000000000000000000000000011
224	00000000000000000000000000000011
225	00000000000000000000000000000011
226	00000000000000000000000000000011
227	00000000000000000000000000000011
228	00000000000000000000000000000011
229	00000000000000000000000000000011
230	00000000000000000000000000000011
231	00000000000000000000000000000011
232	00000000000000000000000000000011
233	00000000000000000000000000000011
234	00000000000000000000000000000011
235	00000000000000000000000000000011
236	00000000000000000000000000000011
RTN	00000000000000000000000000000011
R+C	00000000000000000000000000000011
R-C	00000000000000000000000000000011
R*C	00000000000000000000000000000011
R/C	00000000000000000000000000000011
R^C	00000000000000000000000000000011
R^R	00000000000000000000000000000011
R^C^R	00000000000000000000000000000011
R^R^C	00000000000000000000000000000011
R^R^R	00000000000000000000000000000011
R^C^C	00000000000000000000000000000011
R^R^C^R	00000000000000000000000000000011
R^R^R^C	00000000000000000000000000000011
R^R^R^R	00000000000000000000000000000011
R^C^C^R	00000000000000000000000000000011
R^R^C^C	00000000000000000000000000000011
R^R^R^C^R	00000000000000000000000000000011
R^R^R^R^C	00000000000000000000000000000011
R^R^R^R^R	00000000000000000000000000000011

Binary (\mathbb{A})

RTN	00000000000000000000000000000000
R+C	00000000000000000000000000000001
R-C	00000000000000000000000000000010
R*C	00000000000000000000000000000011
R/C	00000000000000000000000000000011
R^C	00000000000000000000000000000011
R^R	00000000000000000000000000000011
R^C^R	00000000000000000000000000000011
R^R^C	00000000000000000000000000000011
R^R^R	00000000000000000000000000000011
R^C^C	00000000000000000000000000000011
R^R^C^R	00000000000000000000000000000011
R^R^R^C	00000000000000000000000000000011
R^R^R^R	00000000000000000000000000000011

Purely SNS Operators

(Direct Operators)

With (W)

Union (U)

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152
B
E
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L
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N

Purely SNS Operators

Reverse Operators

Reverse or (C)

8. Rearrangement of Logical Equations for Implementations:

We are developing an interactive Software System operating on a set of equations in Matrix Logic for the above purpose. This Software is being written in PASCAL and is executable on the Institute's DEC-1090 computer system.

The Software System basically involves taking in a given set of logical equations via terms, operators, and their connections, as input, and processing this data to produce an ordered set of statements, in which the terms that are initial inputs and final outputs are particularly marked out. The ordered set of statements are written in the required FORTRAN format and they can then be readily taken up for further processing through subprograms already stored in the Computer System.

Being an interactive Software System, it will be possible to stop the forward processing at a convenient stage and reverse along the paths in order to check any argument, if found necessary.

For example, if we have the following set of logical expressions (given in an arbitrary order):

$$\underline{a} \underset{\sim}{\wedge} \underline{b} = \underline{c}$$

$$\underline{c} \underset{\sim}{\wedge} \underline{a} = \underline{y}$$

$$\begin{array}{c} \leftarrow \\ \underline{c} \underset{\sim}{\wedge} \underline{g} = \underline{h} \end{array}$$

$$\underline{c} \underset{\sim}{\wedge} \underline{y} = \underline{k}$$

$$\underline{h} \underset{\sim}{\wedge} \underline{y} = \underline{x}$$

$$\underline{h} \underset{\sim}{\wedge} \underline{k} = \underline{z}$$

These equations correspond to Fig.1 on page 31.

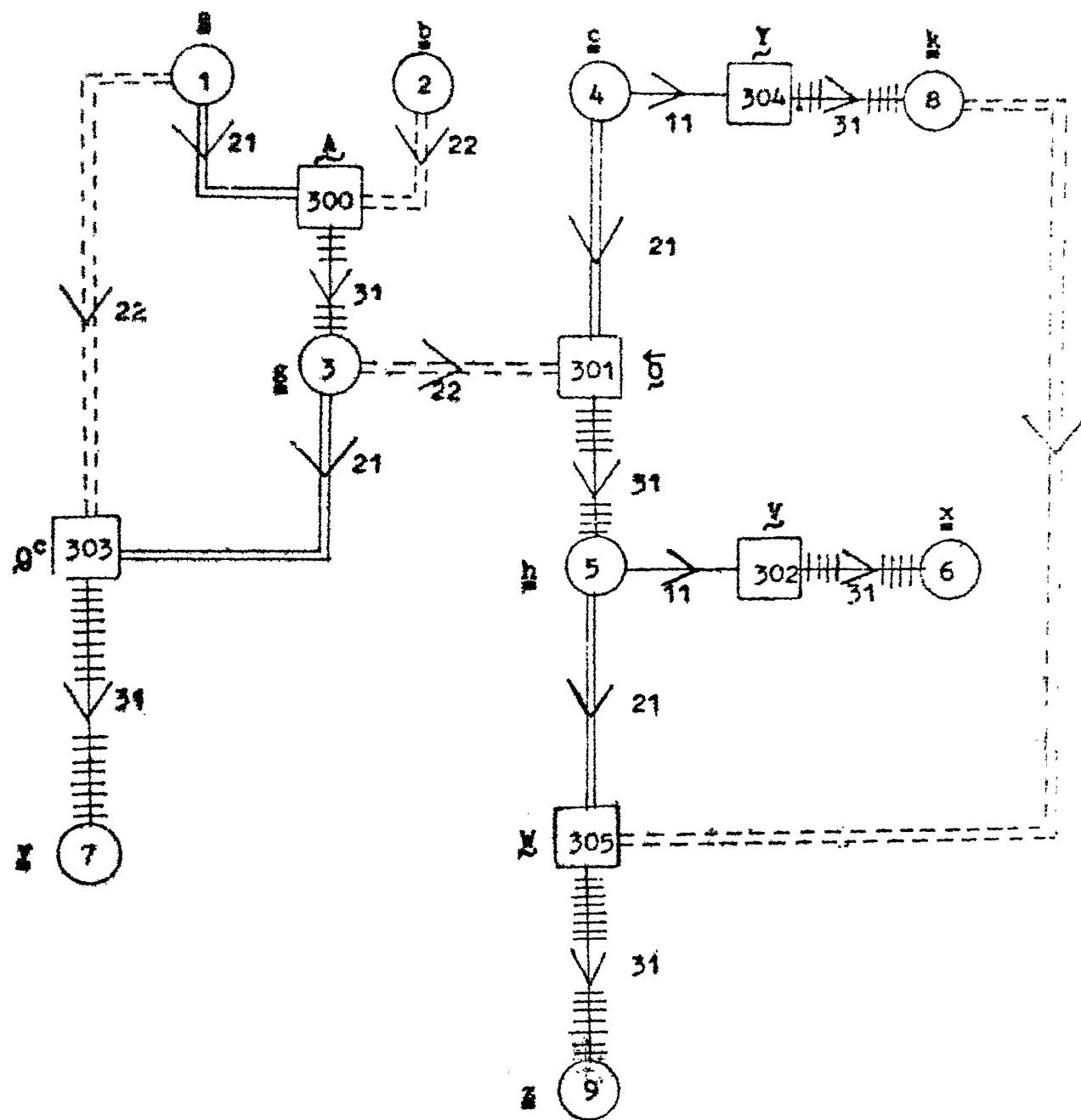


Fig. 1. Typical logical graph used in this study.

Giving numbers and utilizing names (and nature) of terms and operators, the following data are entered into the Computer System when the Software demands it.

Terms:

VAO 1
VBO 2
VGO 3
VCO 4
VHO 5
VKO 8
VXO 6
VZO 9
VYO 7

Operators:

BDN-AE 300
BDN-OM 303
BRN-OE 301
UNN-YE 304
UNN-VE 302
BSN-WW 305

Connector information:

1:(21)300	3:(22)301	301:(31)5	304:(31)8
1:(22)303	3:(21)303	5:(11)302	5:(21)305
2:(22)300	4:(11)304	302:(31)6	8:(22)305
4:(21)301	300:(31)3	303:(31)7	305:(31)9

(Note that within each set of data above the order is immaterial).

After doing this, the following is obtained first:

ORIGINAL INPUTS ARE : 1, 2 and 4.

FINAL OUTPUTS ARE : 6, 7 and 9.

Then the following FORTRAN statements are printed:

```
READ 1, MVAO
READ 1, MVBO
READ 1, MVCO
1   FORMAT(A1)
MVGO = MBDN(MVAO,MZAE,MVBO)
MVYO = MBDN(MVGO,MZOM,MVAO)
MVKO = MUNN(MVCO,MZYE)
MVHO = MERN(MVCO,MZOE,MVGO)
MVXO = MUNN(MVHO,MZVE)
MVZO = MBSN(MVHO,MSWW,MVKO)
PRINT 2, VXO
PRINT 2, VYO
PRINT 2, VZO
2   FORMAT(5X,A1)
```

This output is compatible with the FORTRAN program
MATLOG already developed in our laboratory.

Part II - Fourier transforms of physical functions

Mathematical Theory - S.H.Kulkarni

1. Fourier analysis and its applications

The techniques involving Fourier series and Fourier transforms of a given function constitute what is called 'Fourier analysis'. These techniques can be and are applied to a wide range of problems of physical interest. These problems occur in optics, crystallography, communication theory, tomography, heat conduction, IR spectroscopy etc. Similarly these techniques are applied to many problems of pure mathematical interest that occur in number theory, complex analysis etc. There have been many specialized studies in Fourier analysis from the point of view of applications. Also, there exist a number of treatises on Fourier analysis from the pure mathematical point of view. We have made a few studies in Fourier analysis with an approach, which can be said to lie somewhere in between the two approaches described above, that is to say, we have considered some aspects of Fourier analysis, which will be of interest to both pure mathematicians as well as application oriented persons.

2. Physical functions

We shall define the concept of physical function as follows:

A function $f(x)$ defined on the real line \mathbb{R} is called a "physical function" if it satisfies the following two properties:

- 1) $f(x)$ has a bounded support (BS) i.e, $f(x)$ is identically zero, outside an interval $[-a, a]$.
- 2) $f(x)$ is absolutely integrable (AI) or square integrable (SQI), i.e,

$$\int_{-a}^a |f(x)| < \infty \text{ (AI)}$$

$$\text{or } \int_{-\infty}^{\infty} |f(x)|^2 dx < \infty \quad (\text{SQI})$$

It can be easily seen that under the conditions of Bounded Support, square integrability implies absolute integrability.

The reasons for calling these functions "physical functions" is obvious. If $f(x)$ represents density of an object; then BS means that the object is of finite size and AI means that the object is of finite mass. If $f(x)$ represents an electrical signal, then BS means that the signal is of finite duration in time and SQI means that the signal is of finite energy.

We have considered one-dimensional functions purely for convenience. Most of the analysis can be carried to functions of several variables.

3. Scale invariance

We note that for a function $f(x)$, the manner in which the derivatives $f^{(j)}(x)$ behave with respect to j depends upon the choice of scale for measuring x . This can be demonstrated as follows. Suppose we change x to x' , where $x' = kx$ say. Then the function $f(x)$, expressed in terms of x' becomes $g(x') = f(kx)$, and hence $g^{(1)}(x') = d/dx' g(x') = kf^{(1)}(kx)$. Similarly, $g^{(j)}(x') = k^j f^{(j)}(kx)$. Thus even if $f^{(j)}(x)$ is uniformly bounded for all j , or $f^{(j)}(x)$ tends to some finite limit as $j \rightarrow \infty$, for every x ; we can make $g^{(j)}(x')$ tend to ∞ or 0 by choosing k suitably.

We shall show that, when $f(x)$ is a physical function, it has got many properties which do not depend upon the scale.

4. Infinite differentiability

If $f(x)$ is a physical function, then we define the Fourier transform $F(X)$ of $f(x)$ as follows:

$$F(X) = \int_{-\infty}^{\infty} f(x) e^{i2\pi Xx} dx$$

Since $f(x)$ will have BS, say $[-a, a]$, the above integral will reduce to the following

$$F(X) = \int_{-a}^{a} f(x) e^{i2\pi Xx} dx$$

It has been proved by Paley-Wiener (about fifty years ago) that under the conditions mentioned above (that is, if $f(x)$ is a physical function), $F(X)$ can be defined in the whole complex plane and this extended function say $F(X+iY)$ is an entire function of the exponential type. This means that $F(X+iY)$ is analytic everywhere and

$|F(X+iY)| \leq \alpha e^{\beta|X+iY|}$ where α, β are some positive constant. From this one can easily conclude that the support of $F(X)$ must be unbounded. Or in other words,

"Fourier transform of a physical function cannot itself be a physical function".

We have proved many interesting properties of this $F(X)$, which is the Fourier transform of a physical function $f(x)$. One of these is that $F(X)$ is infinitely differentiable. This means that $F(X)$ has derivatives of all orders and there exist positive constants K and C , such that

$$|F^{(j)}(X)| \leq KC^j \quad \text{for all } X \text{ and for all } j.$$

Thus we see that infinite differentiability is stronger than just the existence of derivatives of all orders or even analiticity. For example, the function $G(X) = e^{-\pi X^2}$ is analytic, but it is not infinitely differentiable.

5. Infinite number of oscillations

Another interesting property of the Fourier transforms of physical function is the occurrence of infinite number of oscillations in the magnitude. This can be described as follows. Let $f(x)$ be a physical function and let $F(X)$ be its Fourier transform. Then for a variety of special cases of $f(x)$, it is possible to prove that one of the following is satisfied.

- (1) $|F(X)|^2$ has infinitely many zeros, and these zeros keep occurring without stop right up to $+\infty$ and $-\infty$.
- (2) $\frac{d}{dx}(|F(X)|^2)$ has infinitely many zeros.
- (3) $\frac{d^m}{dx^m}(|F(X)|^2)$ has infinitely many zeros, for some m .

These results can be used to explain a few empirical facts. If $f(x)$ represents the density of an object, then $|F(X)|^2$ is the intensity of the diffraction pattern. It is an experimentally observed fact, that for any finite object, there are peaks in the intensity of its diffraction pattern. Our result explains the occurrence of these peaks and we can further conclude that these peaks will continue to occur even for arbitrary high frequencies.

Another consequence of the above result is as follows. When we compute the Fourier transform $F(X)$ of a given function $f(x)$, numerically; we always truncate the function $f(x)$ at some stage. The above result shows that this sort of truncation will introduce infinite number of oscillations in $F(X)$. Thus we will never be able to get a monotonic function as the Fourier transform of any function, by a numerical method, however accurate the numerical method be.

M A T H E M A T I C A L P H I L O S O P H Y

(Valedictory Address to the Bangalore
Science Forum, July 31, 1981)

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(Prepared while on leave)

MATHEMATICAL PHILOSOPHY

(Valedictory Address to the Bangalore Science
Forum, July 31, 1981)

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MATHEMATICAL PHILOSOPHY

(Valedictory Address to the Bangalore Science Forum, July 31, 1981).

1. Introduction

The name 'Mathematical Philosophy' would look rather peculiar to many of you, since in the common man's mind, philosophy is associated with vague speculations about the nature of things and such matters. How can one make philosophy mathematical, or, vice versa, talk about the philosophy of mathematics? I hope to show you that both these are possible and that there are some fundamental aspects about reasoning and thinking that can be converted into mathematical terms. I will also show that mathematics itself is not completely self-contained, as many persons think, but that its own nature is subject to a careful philosophical scrutiny. Therefore, my talk today will consist of two parts:

(a) Mathematics of Philosophy,

and

(b) Philosophy of Mathematics.

The two are not similar; but both of them are essential for

any scientist to be a dispassionate observer, analyzer, codifier, and law maker. Since I have had more than 40 years of experience in science, I have taken courage to enter into such metaphysical considerations during the last two or three years; and I shall try, as far as possible, to make these concepts simple and readily understandable by most of you. In fact, the idea is that we will examine the most elementary things that we deal with in mathematics and science, and then consider the relationships between these. In this context, it is to be remembered that such relationships are established only by the application of the human mind, and it is the purpose of philosophy to study "mind", as much as "matter".

2. Philosophy of Mathematics

(a) Natural Philosophy

First of all, we must understand why mathematics is needed, and how mathematics is used, by a scientist in his study of Nature — either as a physicist, a chemist, or a biologist, or in any other branch of Science. The fact that science is an organised system of

knowledge and that it helps man to understand Nature, and even to improve upon the surroundings that he finds himself in, is well-known. So, the first question that we ask ourselves is: How is it that we understand what goes on in nature, and having understood it, how do we write it or preserve it for others to understand what we have discovered? This immediately brings us to several problems — such as the nature of "reason" itself; the relation between reasoning and its statement in a "language"; relation between language, in general, and mathematical language in particular; and so on.

The first one, namely "What is reason?", is beyond the scope of this lecture. I had discussed this to a small extent when I gave a lecture a month ago on 'Philosophy of Science and Religion', wherein I indicated that the ultimate source of knowledge (which is given the name God in religion) is exactly the same as what is given the name "Nature" in science, and which, in Indian Philosophy has the name 'Brahman'. This concept is supposed to encompass everything that exists in nature, not only in their existence and

their characteristics, but also the principles governing their changes and their modifications. Thus, in a naive way, the following may be said: "The same Universal Spirit that makes nature go is also resident in the minds of human beings, and therefore man, even with his limited capabilities, is put in rapport with Nature, and he is able to explain natural phenomena". I am sure there will be hundreds of questions waiting to be asked on this matter; and there are hundreds of different points of view about it. But when they are ultimately analysed, it will be found that the differences are only in matters of terminology and definitions. If one word used by the philosopher, is replaced by another word used by the religious man, or by a third word used by a scientist, and the corresponding explanations are interconverted to one another, it will be found that their semantic contents will be exactly the same. For instance, the subject of physics is itself given the name Natural Philosophy in many British Universities. Newton, for instance, was the Professor of Natural Philosophy, which meant physics, in Cambridge. Thus, science is nothing but the philosophy of Nature, and religion

is nothing but the philosophy of God. Hence, if God and Nature are said to have the same power — scientists say so, for they believe that everything has a "Natural Law" associated with it, and that man only discovers these laws and then proceeds to utilise them — then there is absolutely no place for any conflict between the three disciplines of Science, Philosophy, and Religion.

(b) Qualitative versus Quantitative in Science

Coming now to mathematics as such in Science, why do we need this special branch as an essential component of Science — whether it be the study of physical objects, of chemical changes, of biological processes, or even subjects like sociology and economics? It is needed because, whenever we observe anything, we can talk of two types of relations between one object and another — namely qualitative and quantitative (I am not trying in this lecture to be a strict philosopher and attempt to define everything that I say. Many things, like the words 'qualitative' and 'quantitative' above, are taken for granted and are assumed to have the well known meanings that everybody knows.)

Qualitative relations can be exemplified by statements of the following type: "X is different from Y," or "X is the father of Y," or "if X comes, then the lecture will take place," etc., where no numbers enter the picture. The moment we talk of relations like "X is 1.5 times as tall as Y," "X has 4 children, and each of them has on the average 3 offsprings," etc., we come to the domain of specifications of things in terms of numbers, or mathematical entities. It is a very interesting fact that even non-mathematical statements like those mentioned above can be made mathematical by using a suitable code — this is the essence of representing language on a computer and one employed for machine translation. Even logical relations of a qualitative type can be converted to strict mathematical equations involving matrix algebra, (as we have shown) so that even large arguments in law, or philosophy, can be put into computers, which can then analyse the validity, or invalidity; independence or dependence; etc. of the set of statements in them. Thus, even things which are considered to be qualitative in common

parlance can be rendered quantitative by making use of suitable mathematical techniques. In other words, I can say that there is nothing that man observes and knows, which cannot, in the ultimate limit, be reduced to numbers and equations.

(c) Mathematical Theory in Science

This brings us to the main subject of my discussion today — namely the role played by mathematics in the theories that are postulated in science. As was mentioned above, such theories can be either qualitative or quantitative. An example of a quantitative law is Newton's Second Law of Motion: "Rate of change of velocity is proportional to the impressed force", which can be written in symbols as

$$\frac{dv}{dt} = F \quad (1)$$

This, as everybody knows, requires measurements of time, of distance, and of force, in the form of numbers, and what Eq.(1) says is that the quantity represented on the left hand side in suitable units corresponds to the quantity expressed on the right hand side

in the same units. The principles behind writing such quantitative equations is well known to all of you, and there is no necessity to discuss, in general, about the structure of mathematics, namely how from the very simple concept of integers, one can go to the rational numbers

$$r = n_1/n_2 \quad (2)$$

where n_1 and n_2 are integers, and thereon to the specification of any quantity, however large, or small, it may be, and further on, to the relationship between such quantities, and various mathematical processes that can be applied to them, such as differentiation, integration etc. These details are not essential for understanding the philosophy that we are going to discuss here. It is well realised that mathematics as a subject has a very coherent structure, based on strict logical derivation of one formula, or statement, from another. Hence a result, derived via mathematical processes, is always true, provided there is no mistake in the derivation itself.

On the other hand, not all laws of nature need be necessarily mathematical, at least at first sight. For example, it is a common observation in biology that, if both parents are tall, very often the children are also tall — though this is not always the case. The law: "If both parents are tall, the children are likely to be tall" is, however, only a qualitative law. I am taking this example to indicate two particular aspects of any precise scientific theory. The first is that most theories start off in a qualitative manner, like the above example and then, in course of time, get developed into a quantitative one. In this particular example, it was Mendel, the famous priest-biologist, who gave it a quantitative form. However, as every geneticist knows, this form is ^{also} ~~not~~ deterministic, but only gives the chances of a child being tall or short on the basis of the genetic history of the parents. This is the second aspect I wanted to point out — namely that even the mathematical formulation of a scientific theory need not always be "deterministic", but could be "probabilistic". Thus in genetic theories, the mathematics is not as exact as in Newton's Laws of Motion,

where, given the force as a function of time, the velocity at any instant can be exactly calculated. In genetics, the result is not exact, but only the chances are given. In fact the theory of probability itself is a very important branch of mathematical science, which has been developed to a degree of complication almost comparable to that of deterministic mathematics, in recent years.

From these examples, we see that theories in science generally have three possible structures:

- a) Qualitative,
- b) Quantitative, but probabilistic,
- c) Quantitative and deterministic.

I shall discuss briefly the nature of theories having each of these characteristics and show you that probably something which is a mixture of all three, is in general required in most scientific theories — whether they belong to the domain of physics, chemistry, biology or sociology. This happens because of our limitations of knowledge. As mentioned above, if we do not have enough data, we

can give rough qualitative statements about the phenomenon. When data get acquired more accurately, and the relevant law is determined, it becomes quantitative; but it may be probabilistic, or deterministic. Here we come to a very strange aspect of modern physics — namely that even in physics which is most exact of all sciences, many of the laws that occur, as in thermodynamics and quantum mechanics, are all probabilistic, and determinism that we observe in our observations of nature arises only from the fact that very large numbers of molecules and atoms are contained in any bit of matter that we study, so that the probabilities average out to lead to deterministic equations — e.g. "Rise in temperature of a body is the quantity of heat supplied divided by its heat capacity (product of mass and specific heat.)"

3. Nature of Theories in General

(a) Orderliness in Nature

This brings us to the still more general question of what is meant by a theory. It is almost axiomatic that everything that takes place in nature has some law associated with it. There has

been a lot of controversy in the literature of philosophy as to the origin of this and why nature should be lawful and not completely erratic. For example, the question is asked whether the lawfulness, or order, that we observe in nature is a construct of the human mind and that we observe only those that are orderly and do not notice things which have no relations with one another. However, this cannot be said, and if I may put it in a loose way, the feeling of every scientist is that whatever he studies has an orderly structure, and is based on some theory, or law, in its systematic organisation. In fact, it is the hundred percent belief in the orderliness of Nature (though this may be observable only as probabilistic theories) that makes the scientist go forward. If the scientist finds that one day water is H_2O , and another day it is H_2S , then I am sure he will throw up his hands and say: "I do not want to be a scientist". In fact, the more orderly it is, the more prestige does that branch of science have. It is because the laws governing the behaviour of human beings, and of societies in general, are so much less understood, that these subjects have so

many speculations and so many theories, and so many persons give entirely different descriptions and explanations of the same things.

I shall not consider this aspect much further since in subjects like psychology and sociology, dealing with the understanding of human beings themselves and their behaviour, it is quite likely that contradictory theories are developed by two sets of persons although they are based on the same data. But, even in such cases, if we really go to the root of the question, you will notice that this is only because of the difference in values (i.e. the initial assumptions) adopted by the two sets. In other words, the differences may not even be due to differences in the interpretation of the same thing, but because different items are put into the theory and mixed around to give the results in the two cases.

Leaving aside such difficult subjects, if we take natural science as such, I think there is no doubt that it can be made fully mathematical ultimately. As everybody knows, a good physicist must be a theoretical physicist; a good chemist must be a

physicist, and therefore must know mathematical theory, since that is needed for physics; a good biologist must be a good chemist and should therefore be a good physicist, and therefore, one cannot be sufficiently good in biology unless he has a mathematical instinct in him, although he may not be proficient in actually applying mathematical methods to his specific problems. As I had told you, if anything whatever is thought out, like deducing a consequence from an observation, it is ultimately a mathematical process. Behind the deduction, the author is a scientist at work, and has a whole set of criteria and their interrelations worked out in his mind, before he concludes something about one thing from his knowledge of another one or more things.

(b) Theory of Relations

We just now saw the possibility that, starting from the same set of data, two different theories may be developed; and we attributed this difference to the initial assumptions, or conditions, that are put in not being identical in both the cases. This brings

us to the very general subject of how theory is related to experiment. However, we cannot discuss this generally, unless we go somewhat in detail into an even more elementary concept — namely of the "relation" that exists between two sets of data, or statements. In essence, Science consists of the discovery of such relations, codifying them and analysing and synthesizing them.

Suppose we have one set of data (Set A, consisting of a_1, a_2, \dots, a_m) and from this we deduce certain conclusions (Set B, consisting of b_1, b_2, \dots, b_n). Then, the "science of reasoning" (epistemology) tells us that the first thing to do is to find a 'relation' that connects the first set of quantities a_1 to a_m with the second set of quantities b_1 to b_n , in some unique manner. At present, we are not talking of how one goes about working out the relation; but only of the epistemological principles governing the existence of such a relation. We shall illustrate this by a very simple example. Let a_1 to a_m be the fathers and b_1 to b_n their sons. Then the one and only question we ask is — "Which person

is the son of which father?" As a matter of fact, I have here stated for you the most elementary formula that can be written in the theory of relations, namely the existence, or non-existence of the father-son relationship of b_j to a_i . In general, this can be described by an array of numbers which are all either 1 or 0, as shown in Table 1.

Table 1: Relation between two sets \underline{a} and \underline{b} .

a	b	b_1	b_2	b_3	•	•	b_j	•	b_n
a_1		1	0	0	0	•	•	•	0
a_2		0	1	0	0	•	•	•	0
•		•	•	•	•	•	•	•	•
•		•	•	•	•	•	•	•	•
•		•	•	•	•	•	•	•	•
a_i		0	1	•	•	•	R_{ij}	•	0
•		•	•	•	•	•	•	•	•
a_m		0	0	•	•	•	•	•	1

The meaning of the number 1 at a position (i,j) is that b_j is the father of a_i . In other words, we discuss here a "relation" \sim from set A to set B — namely the condition for b_j being the father of a_i . This can be symbolically stated as follows:

$$\underline{\underline{B}} = (1, 1, \dots, 1) \text{ (n elements)} \quad (5b)$$

We can then denote the relation $\underline{\underline{R}}$ by R_{ij} , which consists of a rectangular array of numbers as in Table 1, where the existence of 1 in the position (i,j) means that the relation R_{ij} is present — which means that the son a_i is related to the father b_j — and $R_{ij} = 0$ indicates that a_i is not related to b_j .

We thus have three quantities — two row vectors \underline{a} and \underline{b} showing which sons a_i and which fathers b_j of the full sets $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are present, and also the standard expression for the relation between the complete set of sons a_1 to a_m (indicated by the vector \underline{a} of (5a)) and the complete set of fathers b_1 to b_m (indicated by \underline{b} of (5b)), which is represented by a rectangular matrix $\underline{\underline{R}}$ whose elements R_{ij} are all only 1 or 0. Now comes the most interesting property. The qualitative idea of the relationship, or 'Relation' as it may be very simply designated, between the sons and fathers may be mathematically represented by the simple matrix equation

$$\underline{a} \underline{\underline{R}} = \underline{b} \quad (6a)$$

which can also be expressed in the vector-matrix form (using Dirac's notation as adopted in quantum mechanics) by the equation

$$\langle \underline{a} | \underline{R} | = \langle \underline{b} | \quad (6b)$$

For those of you who are not familiar with matrix algebra, or the Dirac formalism, I may mention that, effectively, Eqs. (6a) and (6b) lead to the equation

$$\sum_{i=1}^m a_i R_{ij} = b_j \quad (7)$$

It is seen from this Eq. (7) that b_j will be 1 (and the corresponding father b_j will be present in the ensemble), only if the left hand side of (6) leads to a non-zero value.

(c) Boolean Algebra

It must be mentioned that the arithmetic and algebra that we must employ for this purpose is ^{what is} known by the name "Boolean algebra".

The principle is very simple. Boolean algebra deals only with two one-digit numbers, namely either 0 or 1. In Boolean multiplication, (which is indicated by the symbol \otimes), these integers behave exactly as in ordinary arithmetic as shown in Table 2(h). On the other

hand, in addition, the law of addition is given by Table 2(a) which has the following characteristics (\oplus stands for Boolean addition). If both the numbers a and b are 0, then the addition $a \oplus b$ leads to 0; if one is 0 and the other is 1, then the addition leads to 1, all these being exactly as in ordinary arithmetic. The only situation where Boolean algebra differs from ordinary arithmetic is for the sum $1 \oplus 1$ which is also 1. The significance of this is seen from the fact that, if we take 1 as representing existence and 0 as non-existence, adding the condition of existence twice over (viz. $1 \oplus 1$) leads only to existence once again, namely the Boolean number 1.

Table 2: Boolean Addition and Multiplication

(a) $a \oplus b = c$

a	b	1	0
a			
1		1	1
0		1	0

(b) $a \otimes b = c$

a	b	1	0
a			
1		1	0
0		0	0

The application of Boolean addition and multiplication in the context of our problem, namely of existence and non-existence,

is very simple. Addition $a \oplus b$ means that if either "a or b" (or both) are present, then c gives the value 1 corresponding to the presence of either of them. For the multiplication $a \otimes b$, on the other hand, the simultaneous presence of both is necessary to give the value 1 for $c = a \otimes b$. If either is absent (i.e. a or b is 0), then the "a and b" does not exist, and is zero. In fact, these two concepts are absolutely vital for the subject of Mathematical Logic; and almost everything in logic can be proved from just these two concepts, and one more, namely that 0 and 1 are exclusive states standing for absence and presence of a property and that the negation of one leads to the other. This last is what is done in the Boolean vector representations $\langle a \rangle$ and $\langle b \rangle$, and in the Boolean matrix representation of $|R|$.

If we remember all these, then the interpretation of Eq. (7) becomes obvious. If in the product $\sum_i a_i R_{ij}$ there is at least one product $a_\alpha R_{\alpha j}$ which is unity because a_α is present and the relation $R_{\alpha j}$ also exists, so that it has a value $1 \otimes 1 = 1$, then $b_j = 1$. This means that if any one of the sons is related by the

relational matrix to the father b_j , then among the sons (Set a) of the ensemble, as given by (4a), there is at least one person who is related to b_j as being his son, and b_j is a father of one son in the set a. In other words, Eq. (7) can even be utilized for the procedure of picking out (from out of the full set B represented by the vector B), the related ensemble of fathers b, when the ensemble of sons present (namely a) is given.

(d) Forward and Reverse Relations

In essence, the theory of relations briefly discussed above deals with the problem of "How is set a related to set b" and this forward relation from set A to set B is given by the elements of the matrix R_{ij} . In other words, what was originally stated as a set of qualitative relations — namely "Mr. b_4 is the father of Mr. a_m " etc. — is converted into a mathematical formula. The beauty of this formula is that, many rules and procedures of a much more advanced branch of mathematics (namely linear matrix algebra) can all be taken over to represent and work out qualitative relations like 'yes', 'no', 'and', 'or', 'if', etc. Thus, given a "forward"

relation $\underline{a} \sim \underline{R} = \underline{b}$, we may ask about the "reverse" relation from \underline{b}

to \underline{a} . In our notation, we represent this reverse relation by $\overleftarrow{\underline{R}}$,

and mathematically, we may represent it in the vector matrix formalism as follows, by using a suitable matrix $|\overleftarrow{\underline{R}}|$:

$$\underline{b} \overleftarrow{\underline{R}} = \underline{a} \quad \text{or} \quad \langle \underline{b} | \overleftarrow{\underline{R}} \rangle = \langle \underline{a} | \quad (8a)$$

It means that \underline{b} is related to \underline{a} by the relation $\overleftarrow{\underline{R}}$, as a consequence of the fact that \underline{a} is related by \underline{R} to \underline{b} . The table corresponding to $\overleftarrow{\underline{R}}$, similar to Table 1 for \underline{R} , is obviously seen to be obtained by interchanging the rows and columns of Table 1. Consequently, the elements of the matrix \overleftarrow{R}_{ij} are readily seen to be given by

$$|\overleftarrow{R}_{ij}| = *|R_{ji}| \quad (8b)$$

It should be pointed out that the "reverse" matrix is entirely different from the so called "inverse matrix" defined in Linear Matrix Algebra, where the inverse cannot be formulated unless $m = n$. However, the condition $m = n$ is not at all necessary in this particular discipline of the theory of relations, and the "reverse" relation is representable by $|R^t|$ (transpose of the

matrix $|R|$). Thus, in Eq. (8a) we have

$$|\overleftarrow{R}| = |R^t| \quad (8c)$$

We shall read \overleftarrow{R} as "reverse R ".

The above ideas are not found in most books on algebra. They are to be found, instead, in text books on logic, and those dealing with Boolean algebra. The use of Boolean arithmetic and algebra has led to greatly simplified procedures in the practical applications of logic, particularly in Computer Science.

(e) Qualitative versus quantitative relations

We have already seen that the Laws of Nature can be either qualitative or quantitative and that, when they are quantitative, they can be either probabilistic, or deterministic. Just now, we saw how qualitative relations, where we only say that a relation exists, or does not exist, can be given a mathematical representation via the algebraic theory of relations, using Boolean matrix algebra. It should be noticed that, although I use the word "qualitative", which means that you could only ask two questions

"Is it?", or "Is it not?", it is possible to answer even questions like "Is it all?", "Is it some?" or "Is it none?" by suitably modifying the above algebra, and build up another type of qualitative value for relations, other than just "yes" or "no". This is used in the so-called first order "quantified" predicate logic. Please look at the contradiction in terms — namely the use of the word "quantified", which is done because we decide between all, some or none — while technically, each is only a "qualitative" possibility with no numbers entering the picture, and we only comment on whether , all of a is related to all of b, or to some of b etc. In the same way, we can have any number k, of different qualities for a and similarly, l different qualities of b, and use the theory of the previous subsection to give a theory of the relationships between these (just like the father-son relation). We shall not discuss this any further, except to point out how exceptionally simply logic can be handled in terms of these algebraic ideas. We shall mention some of these in the next section.

Considering, instead, quantitative relations, we shall first

discuss the probabilistic type of relation between two properties a and b, and show formally that it is closely related to the above theory of relations. For example, we may compare the quantitative relation between the number of persons having their heights varying between 5 ft and 6 ft, at intervals of 3 inches and similarly, of their weights varying between 100 and 200 pounds, at intervals of 20 pounds. Then one gets a table similar to the one shown below:

Table 3: Probability relations between height and weight*

h_i	w_j	w_1 100-120	w_2 120-140	w_3 140-160	w_4 160-180	w_5 180-200	Total (a_i)
h_1 5'0"-5'3"	4	6	5	1	0	16	
h_2 5'3"-5'6"	7	14	8	6	0	35	
h_3 5'6"-5'9"	6	10	12	4	1	33*	
h_4 5'9"-6'0"	1	2	4	7	2	16	

* The table gives fractions P_{ij} (in percent) of those having the height and weight in the range (h_i, w_j).

+ To calculate the fraction (f) required in the text, we have

$$f = P_{32} / (\sum_j P_{3j}) = 10/33 = 30\%$$

This 4 x 5 table in fact contains as entries, the percentage of cases which have the combined property of having the height interval

within h_i and the weight interval within w_j . This table can be constructed by anyone who has access to, let us say, the required data for all the students of a college. Now we can ask the question, "Suppose the height of a student is given to be between 5'3" and 5'6"; what is the probability that his weight is between 120 and 140 pounds?" I won't write the equation, but you will readily see that all that is necessary is to take the row marked in the table, which corresponds to all possible cases w_j ($j=1$ to 5) having also their heights between 5'3" and 5'6", and then take the square marked, which picks out of this the value corresponding only to those having the weight range between 120 and 140 pounds. Then, if all the numbers in the row are added, and the number in the square divided by this, the ratio gives the fraction f that has the double property (h_i, w_j) among those having the single property h_i (see Table 2 bottom). By very simple arguments like this, various results in probability can be worked out. The purpose of this discussion is merely to point out that the probabilistic relationship between h and w is representable as a rectangular array P_{ij} , which is very similar to R_{ij} of the last section, except that the P_{ij} 's are now percentages, having all possible values between 0 and 1 (corresponding to 0% and 100%), and not only the two Boolean numbers 0 or

1, which occur in R_{ij} . The algebra of using this matrix is slightly different from what was mentioned earlier for R_{ij} because standard linear algebra, and standard arithmetic, have to be employed, instead of Boolean arithmetic; but the essence of the argument, namely that the relationship between \underline{h} and \underline{w} is representable by a rectangular matrix remains. Just like Eqs. (3) and (6), we have now the formulae:

$$\text{Probabilistic relation } \rightsquigarrow : h_i \xrightarrow{P_{ij}} w_j \quad (9a)$$

$$\sum_{i=1}^m a_i P_{ij} = b_j \quad (j=1 \text{ to } n) \quad (9b)$$

It is important to realize that, although we use standard arithmetic for obtaining the "reverse" probabilistic relation $\overset{\leftarrow}{\rightsquigarrow}$ it follows the structure of our Theory of Relations, and not linear algebra, and we obtain for this the following:

$$\overset{\leftarrow}{P} : w_i \xrightarrow{P_{ij}} h_j ; |\overset{\leftarrow}{P}| = |P^t| \quad (10a)$$

and

$$\sum_{i=1}^n b_i \overset{\leftarrow}{P}_{ij} = a_j \quad (j=1 \text{ to } m) \quad (10b)$$

4. New ideas in Logic

I have spent so much of time in talking about relations in general, because it is well recognised that qualitative ideas in

logic, such as "a is the same as b", "a is the opposite of b", "if a is true, then b is true", "a and b cannot both be true", etc. form the essential basis of the steps in an argument dealing with everything in science, and, in particular, of everything in mathematics. Usually, these are taken for granted, by saying that a person who can think clearly can obviously also think logically. This is of course true so long as the argument is not too complicated. We know of famous lawyers who can twist an argument in such a way as to make it highly plausible, and make one believe that a certain thing had taken place, while a very careful detailed analysis may in fact show that it did not at all happen. The flaw in the argument can be shown only by another lawyer, who is equally or more intelligent than the former.

Obviously, we do not want such a situation in mathematics; one mathematician should not hoodwink another. We should see that any mathematics that is correct could be checked to be so by everybody, and tests should be available to show whether they agree with

accepted norms of thinking. This is the subject of logic. It is a very old subject and existed more than 2,000 years ago; and it is interesting to note that practically all the basic principles had been enunciated by the Greeks, and to a smaller extent, also by Indian logicians. The Indian logicians had an intuitive approach, while the Greeks had an analytic approach — it is not for me to say which of these two is more useful, although the former may serve the purpose in many cases. Modern mathematicians believe that analytic proofs of everything is absolutely necessary, and that one can never accept a result simply because it fits everything that is needed, unless the rootcause and the derivation of it are stated in unmistakable terms. This is certainly a very highly desirable ideal; but only an ideal. I shall indicate reasons to believe that, even in pure mathematics, this ideal has not been completely achieved.

(a) Deduction

To show this, I will discuss the subject of logic in some

detail, and show you how from very simple general considerations, we can show that logic cannot have any flaws in its structure, provided we try to achieve this in the proper way. You would imagine that this statement is not necessary; but I am saying this because there is a well-known theorem in logical science, due to the famous mathematician Kurt Gödel, which says that a set of sentences, having various logical interconnections between them, cannot be built which is completely self-consistent and complete, if all their consequences are taken into account. I am putting the theorem in a very crude way. I think it is called the "Incompleteness theorem of theories", indicating that everything that can be said about some subjects cannot be derived from a finite set of axioms.

We shall therefore examine how we should set about so as to be able to say, at any time, that the statements in a theory form a self-consistent set, and that there are no contradictions between one statement and another. In fact, if we cannot do this, we cannot prove any theorems in mathematics, because many theorems

in mathematics are proved by what is known as the "reductio ad absurdum proof", in which we assume the contrary of what is to be proved and show that it leads to a contradiction with some well known fact, or theorem, and use the impossibility of a contradiction to deduce that the contrary of the theorem is wrong, and therefore that it is correct.

The above technique has two parts to it. One is that we should be able to have strict rules to say exactly when there is contradiction, and when there is consistency and absence of contradiction. If this is possible, we can proceed to the second step. In this, a well-known theory, or set of statements, which is completely selfconsistent is taken to be available. Then, if a new statement, say S, is added to it, and it is found to be inconsistent with, or contradictory to, one or more of the statements in the theory, then the new statement S must be wrong, or invalid. Even with the use of our crude words, this can be seen to be true by any thinker. If something contradicts a well known

thing, then that new statement must be wrong.

On the other hand, to prove something is right is a very much more difficult problem. It is not enough to show that it is consistent with everything that is known; but it is necessary to show that it is derivable, or deducible, from one or more facts, or theories, that are already known; and also that it is not inconsistent with everything that is known. The first part is very good, and everybody agrees that

If $\underline{a} \Rightarrow \underline{b}$ and \underline{a} is true, then \underline{b} is true.

This is a famous method of syllogism used by the Greeks and widely used in Indian logic (Dhumāt vahnīḥ — smoke implies fire).

This can be put in several different forms, but we shall only examine this one form. In this example, \underline{b} can be deduced to be valid, if \underline{a} is valid. Now, if we know that \underline{a} is not inconsistent with the theory, or the domain of knowledge that we presently have, does it not necessarily follow that \underline{b} is not inconsistent and is perfectly valid? I think it is so. Thus, if \underline{b} is deduced from \underline{a} , and \underline{a} is not inconsistent with

all that is known, then it is not necessary to prove once again that b is consistent with everything. This is what makes life possible for a mathematician, or a scientist.

(b) Paradoxes

Unfortunately it is not such an easy life as all that. In rare cases, we find in some other way that b is inconsistent with something. Now, such cases are extremely rare, but examples can be built of special arguments where such a paradox occurs. The word "paradox" may be explained by saying that, in it, we come to the strange conclusion that something is true by one method, while we get it to be false by another method; and we are unable to find out any reason, why this peculiar impossible combination should occur. The question is often asked "Should logic admit paradoxes?" and you will be surprised to learn that the accepted formalism of logic says there will always be paradoxes in most theorems.

Let us examine this statement — "A logical system will not

be free of paradoxes". If this is so and paradoxes are admissible in logic, when does one say that a contradiction means that the statement leading to it is invalid, and when does one say that the contradiction leads to a paradox? Yet, there are paradoxical statements, which are perfectly admitted by standard logical systems. I believe that the very admission of paradox in logic — namely that a contradiction can be permitted without affecting the structure of the theory itself — is illogical and invalid, unless rules are available to decide as to when a certain logical difficulty found is a paradox and can be accepted, and when it is a contradiction and is unacceptable. Such a rule is available in certain systems of logic, in which paradoxes are admissible for a statement that comments on itself — e.g. "What I say is untrue" and such statements are excluded. We shall not discuss this further.

Thinking about this, we have developed a theory in which we have definite rules for detecting contradictions, which incidentally are quite consistent with the rules of standard logic. But

we go further and say that a contradiction always leads to the result that something is invalid. You can never accept an argument that is contradictory. This is fully in line with the standard method of reductio ad absurdum, where a contradiction is in fact utilized to prove the opposite of a result.

Therefore the question arises — What if a result and its opposite both lead to contradictions? Is it a paradox? To illustrate this, I will take one classical example, which is commonly accepted as being a paradox — namely that of the Cretan liar mentioned above. He says, "What I say is false", and the question is asked "Is this sentence itself true or false?" You can easily see that if it is true, then by the content of the sentence it must be false. And if it is false, then it follows from the sentence itself that it must be true, and we arrive at a paradox Our answer to this is very simple. There is no Cretan liar. In effect, a sentence like this is inadmissible in our system of logic. In other words, we have a rule which takes a

series of steps to check the consistency, or otherwise, of a new statement with the set of statements already known and if it does not satisfy these tests, then it cannot be included in a valid logical argument. In fact, we can write a computer program in our logical system, which will print 20 question marks when the Cretan liar statement is fed into it, indicating that it is inadmissible. If a computer can be made to reject all contradictions, then you must accept that it does not depend upon how any particular statement is looked at, but is the consequence of the system that we have developed. In our system, there are no paradoxes, and if any argument leads to a paradox, the source of this is traced and thrown out.

I am sure many of you will be highly skeptical of all that I have said. But, I was happy to note that the famous mathematician M.H. Stone, who was here in Bangalore, was quite agreeable to our methods and approaches, although he said that he was not a specialist in logic. But he did say that "There are so many systems of logic floating about, that adding one more, which you believe has

some advantages, is certainly permissible."

(c) Some matrix algebraic aspects

We shall indicate briefly how the Theory of Relations we had discussed in Section 3 could be used for converting propositional logic into a computerizable matrix-algebraic form, using Boolean addition and multiplication. The principle is as follows. Just as in Table 2, we now take two statements \underline{a} and \underline{b} , each of which has two possible mutually exclusive states, "true" (a_α and b_α) and "false" (a_β and b_β). Thus we express the truth state of a general statement \underline{v} by the vector $\underline{v} = (v_\alpha \quad v_\beta)$, where v_α , v_β are both 0 or 1. Then, we make the following identifications:

$$\text{True} \equiv \underline{v_T} = (1 \quad 0) ; \text{ False} \equiv \underline{v_F} = (0 \quad 1) \quad (11)$$

To obtain the matrix of the transformation from \underline{a} to \underline{b} via a logical relation say "not" — we first formulate its corresponding truth table (as routinely used in standard logic), as in Table 4(a). This table is obvious and requires no comment and the relational matrix $|N|$ derived therefrom is shown below the Table 4(a). Then,

Table 4: Logical Truth Tables for "Not" and "Implies"

$$(a) \underline{a} \text{ } N = \underline{b} \quad (\neg \underline{a} = \underline{b})$$

\underline{a}	\underline{b}	1	0
\underline{a}			
1		0	1
0		1	0

$$(b) \underline{a} \text{ } I = \underline{b} \quad (\underline{a} \implies \underline{b})$$

\underline{a}	\underline{b}	1	0
\underline{a}			
1		1	0
0		1	1

$$|N| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$|I| = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

If the input \underline{a} is true (1 0), or false (0 1), we have the following equations leading to \underline{b} being false and true respectively as a result of the negation:

$$\langle a_T | N | = (1 \ 0) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (0 \ 1) = \langle b_F | \quad (12a)$$

$$\langle a_F | N | = (0 \ 1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (1 \ 0) = \langle b_T | \quad (12b)$$

In fact everything that can be conceived about, or done with, the logical connective "not" (or "negates"), is contained in the matrix $|N|$ of Table 4(a), applied as per Eqns. (12a) and (12b).

In the same way, the implication $\underline{a} \implies \underline{b}$ is readily seen to be given by the matrix $|I|$ of Table 4(b). In this case, we

have, analogous to (12a) and (12b), the following equations

$$\langle a_T | I \rangle = (1 \quad 0) \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} = (1 \quad 0) = \langle b_T | \quad (13a)$$

$$\langle a_F | I \rangle = (0 \quad 1) \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} = (1 \quad 1) = \langle b_D | \quad (13b)$$

$$b_D = b_T \oplus b_F = (1 \quad 0) \oplus (0 \quad 1) = (1 \quad 1) \quad (13c)$$

It is clear that $\underline{a} \implies \underline{b}$ requires that a_T always leads to b_T .

On the other hand, when \underline{a} is false (a_F), we know that "both b_T

and b_F are possible", which is expressed in our notation by b_D

(D = doubtful) which is the Boolean sum $b_T \oplus b_F$.

Thus, in the extension of propositional logic that we have

developed, new states of truth are introduced in addition to the

states $\underline{T} = (1 \quad 0)$ and $\underline{F} = (0 \quad 1)$, and there are two more states

possible, namely doubt $\underline{D} = (1 \quad 1)$ and contradiction $\underline{X} = (0 \quad 0)$.

The meaning of the "doubtful" state \underline{D} is clear from the above example,

and is the Boolean sum $\underline{T} \oplus \underline{F}$. It means that either the true state

or the false state is possible under the circumstances. In the

same way, it is possible to define \underline{X} as the Boolean product of the

states T and F as follows.

$$\underline{\underline{T}} \otimes \underline{\underline{F}} = (1 \quad 0) \otimes (0 \quad 1) = (0 \quad 0) = \underline{\underline{X}} \quad (14)$$

This means that simultaneously the statement concerned is both true and false, when it is in the state X. Since, in our logic, the two states T and F are mutually exclusive, both together cannot occur; hence we call the state $(0 \quad 0)$, = X, as the "contradictory" state. In actual practice, if a logical argument, on computerization, leads to the state X at some step, then it means that during the earlier steps of the argument two mutually contradictory statements have been introduced. We have, in fact, worked out procedures whereby such contradictory statements could be traced back and identified.

There is no time to show how exactly all the various other connectives in logic are worked out, in terms of the vector-matrix formalism. Thus, in classical logic, in addition to the "unary" relations of the type shown in Eqs. (12) and (13) for N and I, we can have also "binary" relations of the type $\langle \underline{a} | R | \underline{b} \rangle = c$. The entity c (in this case) is a number, but it can be converted

into a state vector $\langle c \rangle = (c_\alpha \quad c_\beta)$, by identifying the Boolean values $c = 1$ and $c = 0$ with the vectors $\langle c \rangle = (1 \quad 0)$ and $\langle c \rangle = (0 \quad 1)$. We shall not discuss this further, since it becomes highly technical, and should be reserved for a detailed scientific discourse than for a popular lecture.

In a very brief way, we may mention similarly that if three-element vectors are taken and we denote such a vector α by $(a_\gamma \quad a_\delta \quad a_\epsilon)$, then the various possible quantified states can be represented. Obviously, eight possibilities exist, if the three Boolean elements $a_\gamma, a_\delta, a_\epsilon$ have each the two possibilities 0 and 1. However, out of these, only four are commonly used — namely the following:

$$\begin{aligned}\forall &= (1 \quad 0 \quad 0) — (\text{For all}) \\ \neg \forall &= (0 \quad 1 \quad 1) — (\text{Not for all}) \\ \exists &= (1 \quad 1 \quad 0) — (\text{There exists}) \\ \emptyset &= (0 \quad 0 \quad 1) — (\text{For none})\end{aligned}\tag{15}$$

However, similar to the D and X states in propositional logic, we can also have two other states

$$\Delta = (1 \ 1 \ 1) \text{ and } \times = (0 \ 0 \ 0) \quad (16)$$

which correspond to complete doubt (Δ) and impossibility (\times).

We shall mention nothing further, except to point out that the vector-matrix formulation thus has immense possible applications in quantified logic also.

(d) Some esoteric aspects

This is the right place for us to consider certain esoteric aspects connected with logic. Thus, one asks the very general question, "Is knowledge always attainable about everything in nature?" The question is not regarding practical matters; obviously one has to go on finding out more and more about everything, and man's life is certainly too short for him to exhaust the study of all aspects of Nature. However, we may ask the question whether, given sufficient time and facilities, it is possible to know everything about some thing. The emphasis is on knowing completely about some one thing, rather than knowing about all things that are present. In other words, is complete knowledge obtainable, in

theory, about every object; or are there some things about which full knowledge cannot be obtained? This is not a silly question, because, as we have seen in the last section, even some mathematical theories can be shown to be not capable of being made complete.

Theoretical knowledge about any subject is, ~~in general~~, never 100 percent complete. In fact, the great mistake that the 19th century scientists (in particular physicists) made was to believe that the number of fundamental laws that have to be formulated to cover the whole field of physics will be limited. However, a simple analysis of the process of obtaining theoretical knowledge shows that it is a continuously repeating process, that every new fact that is determined has to be shown to be completely consistent with the known theory, and that there is nothing that one definitely knows which can show that no new fact will be found which does not fit the existing theory. In other words, nobody can ever prove that the complete theory of something has been worked out. Nature is a beautiful woman, but a very elusive one, one who always runs away from your grasp when you think that you have caught her and

understood her.

Apart from this aspect of epistemology, I would like to draw your attention to another one which was the centre of attention in Ancient Indian Philosophy. According to Indian Philosophers, the sum total of knowledge was pictured as the embodiment of the Supreme Being that is responsible for "all this world going around" (Yena bhrāmyate brahmacakram). The question that they asked was — although we may try to understand all that takes place, and try to understand the reason for these, can we understand completely the nature and extent of the Supreme Being itself, which is the ultimate cause of everything? It is rather interesting to note that they were extremely careful about answering this question. For instance, in the Kena Upanishad, (in which the word 'Kena'? means "By whom?" or "By what agency is Nature governed?"), they answered the above question only by means of paradoxical statements. Many western scholars scoffed at this way of writing — for example

Yasyamatam tasya matam matam yasya na veda sah
(He who knows it, does not know it ; he who does not
know it really knows it.)

It is usually left off, saying that it is a conundrum or a puzzle of words, and is of no great significance. But I want to point out that it is the one and only way by which we can describe the Supreme Being — namely that He is neither understandable nor non-understandable — that is, "He is beyond understanding". If we think that we have understood It (Nature), we are wrong; but if we can realise that It can never be understood, then we have achieved the true understanding of it.

In logical terms, we thus have

$$(\neg \underline{a}) \text{ Not understood} = (\underline{a}) \text{ Well understood} \quad (17)$$

— clearly a paradox; but I wish to say that this paradox is not a contradiction. I shall prove it from logic. If, to the question 'Can I understand it?' you answer 'yes' (say a_T), then the above Eq. (17) is a contradiction because a_T is put equal to a_F . If you answer it as 'no', then also it is a contradiction, because Eq. (17) leads to the result that a_F is equivalent to a_T . But if you give the answer 'I cannot say' or 'I do not know', then there

can be no contradiction coming out of it, for we then have $a_D = (1 \quad 1)$.

You can only know that you can never know everything about this supreme entity. As a matter of fact, in our system of logic with \underline{D} state included, we find that a proposition can be equivalent to its negation only if it has the state $\underline{\underline{D}}$. In fact,

$$\langle a_D | N \rangle = (1 \quad 1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = (1 \quad 1) = \langle a_D | \quad (18)$$

This means that if the statement can take either of the states \underline{T} or \underline{F} , and we are not in a position to say which it is, it cannot be contradicted by negation. Thus, if one can never know whether something is true or false, the exact opposite of it is also the same, namely that one can never know whether it is false or true. Therefore the concept as given in the Ancient Upanishads of India of the Supreme Being is not a paradox. It is permitted by logic so long as no definite information about it is ever capable of being obtained. This is in fact exactly what the Kena Upanishad emphasises again and again. It says in one place, 'I think I have understood it', but again 'I am afraid, I do not know'. Again it says 'Known

to the unknown, unknown to the known', and so on. These are not play of words; they contain, in fact, the most supreme concepts, and perhaps this is the one and only definition of what, in every religion, is known under the name "God".

(e) Back to terra firma

From these olympean heights, we will now come down to more mundane aspects, and talk about some possibilities that arise out of this doubtful state commonly in arguments and debates. Before that, let me explain that we use the contraction SNS for our logic. It stands for the words Syād Nyāya System — in which 'syād' means 'may be' and 'nyāya' means 'logic'. This "may be" system was originated by the Jains in India in the B.C's and they held that, before we get definite knowledge, everything is vague and uncertain, and lies in the syād state. We can only say: "It may be true, or it may not be true", and the Jains postulated that the process of gaining 'Jnāna' or 'knowledge' was by the fact that the syād state is removed and the definite state is induced. In logic, the definite state will be either true or false, about any property

of the system.

On the other hand, as mentioned above, if we do not know whether something is true or false, then it can never be contradictory, and hence can never be proved to be wrong. This is the greatest boon to our administrators and politicians. When they want it to be such that they are never found fault with, the only method is not to take any decision — simply say "May be", or "We shall see", or some such. They can never be found to be in error and as we all know to our desolation, this is exactly what is adopted by all the great rulers in our country. So, I can close this lecture with the happy thoughts that I have given full marks for the Technique of Universal Procrastination, which is the keynote of our administrators!

I N T E R I M P R O G R E S S R E P O R T O N
T H E L O G I C M A C H I N E
Q U A N T

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1. Introduction

The machine QUANT has been developed for working out problems in Predicate Logic, just as ESNY was developed for Sentential Logic. The essential new feature that has made this machine possible is the representation of quantifiers by means of 3-element vectors $(\gamma' \delta' \varepsilon')$ analogous to the 2-element vector $(\alpha \beta)$ of propositional calculus. (The dashes in $\gamma', \delta', \varepsilon'$ are used to distinguish them from similar 3-vectors $(\gamma \delta \varepsilon)$ which will be defined later for a new "canonical form" of the quantified statement (QS), which appears to be the suitable form for manipulations in predicate logic using the vector-matrix formalism). Thus, the quantifier in QUANT has 3 electrical lines $\gamma', \delta', \varepsilon'$ to represent the quantifier, in addition to 2 lines α, β to represent the proposition that is quantified. As will be seen below, one more line ζ is needed to indicate the positive (affirmative) form or the negative form of the quantifier. These lines are all coded by standard TTL voltage levels, viz., 0 V and 5 V, representing 0 and 1 of the corresponding Boolean element of the vector. This coding is used for all the 6 lines $\alpha, \beta, \gamma', \delta', \varepsilon', \zeta$.

Considering the quantifier only, the classical ones are \forall (for all), \exists (there exists), Λ ($= \neg \forall$, not for all), and \emptyset (for none). It so turns out that these are not the basic states (which are independent) for a 3-element Boolean vector system. Since there are three elements, namely $\gamma', \delta', \varepsilon'$, it is natural to take the states $(1 \ 0 \ 0)$, $(0 \ 1 \ 0)$ and $(0 \ 0 \ 1)$ as the basic states. It can be shown that the standard forms of quantified logic can all be represented in terms of these three, which may be denoted by "For all", "For some" and "For none" (see Table 1). Then, it follows that

Table 1. Quantified States

Boolean elements			Nature of State	Name
γ	δ	ε	Symbol	
1	0	0	\forall (std)	For all
0	1	0	Σ	For some (only)
0	0	1	\emptyset (std= $\neg \exists$)	For none
0	1	1	Λ (std= $\neg \forall$)	Not for all
1	0	1	Θ	For all or none
1	1	0	\exists (std= $\neg \emptyset$)	There exists
0	0	0	\times	Impossible
1	1	1	Δ	Indefinite

the two other states $\exists V (= \Lambda)$ and $\exists (\neg \emptyset)$ are the negated forms of the states V and \emptyset . These are shown in rows 4 and 6 of Table 1. It is then obvious that one more negated state will occur, viz., $\exists \Sigma$ (Not "for some"), which can be given the simple name "For all or none" (See Table 1). In addition to those, there are two more possibilities, to make up the 8 ($= 2^3$) possibilities for a 3-element Boolean vector. We shall designate these by the symbols $(0 \ 0 \ 0) = *$ (Impossible) and $(1 \ 1 \ 1) = \Delta$ (Indefinite). The occurrence of the impossible state or the indefinite state in quantified logic can be explained in exactly the same manner as the occurrence of the X and D in SNS logic. The following formulae are readily verified:

$$V \oplus \Lambda = (1 \ 0 \ 0) \oplus (0 \ 1 \ 1) = (1 \ 1 \ 1) = \Delta \quad (a)$$

$$\emptyset \oplus \exists = (0 \ 0 \ 1) \oplus (1 \ 1 \ 0) = (1 \ 1 \ 1) = \Delta \quad (b)$$

$$\Sigma \oplus \Theta = (0 \ 1 \ 0) \oplus (1 \ 0 \ 1) = (1 \ 1 \ 1) = \Delta \quad (c)$$

$$V \otimes \Lambda = (1 \ 0 \ 0) \otimes (0 \ 1 \ 1) = (0 \ 0 \ 0) = * \quad (d)$$

$$\emptyset \otimes \exists = (0 \ 0 \ 1) \otimes (1 \ 1 \ 0) = (0 \ 0 \ 0) = * \quad (e)$$

$$\Sigma \otimes \Theta = (0 \ 1 \ 0) \otimes (1 \ 0 \ 1) = (0 \ 0 \ 0) = * \quad (f)$$

The significance of the Boolean sum and the Boolean product, in Eqns (1a) to (1f), is identical with what is done in SNS logic, viz., the concurrent, or alternative, possibilities of the two states that are added being designated by \oplus , and the product \otimes standing for the simultaneous existence of both states. It is then obvious, from the fundamental principles of our matrix representation, that a state and its negation both being likely leads to complete lack of information, i.e. indefiniteness, or doubt, represented by the quantified state Δ as in (1a,b,c). Similarly, the simultaneous occurrence

of a state and the negation of the state is impossible in standard logic, in which it is asserted that anything must be either true or not true, and cannot at the same time be both true and not true. Hence the three possibilities in (1d,e,f) lead, by Boolean multiplication into the 'impossible' or 'contradictory' state, that is designated by *.

In addition to the $\gamma', \delta', \varepsilon'$ components, we also use the element ζ , which has the role of being used to represent the "YES" or "NOT" which qualifies the quantifier. When $\zeta = 0$, it is read as "not"; otherwise there is no qualification specifically mentioned. Thus, when $(\zeta) (\gamma' \delta' \varepsilon')$ is (0) (1 0 0), it is read as "not for all", and when it is (1) (0 0 1), it is read simply as "for none". Thus the six elements of a quantified statement,

$$QS; \quad (\zeta) (\gamma' \delta' \varepsilon') (\alpha \beta) \quad (2)$$

represent a general quantified statement, where $(\zeta) (\gamma' \delta' \varepsilon')$ is the standard "quantifier" and $(\alpha \beta)$ constitutes the SNS state of the statement quantified by it.

Of the eight quantifiers listed in Table 1, the first three, viz. \forall , Σ , \emptyset , are designated as "pure" (basic) quantifier states, and the remaining ones can be obtained from these three by making "combinations" (Boolean sums) of these. Thus,

$$\forall \oplus \Sigma \equiv \exists \quad \emptyset \oplus \Sigma \equiv \Lambda \quad (3a)$$

$$\forall \oplus \emptyset \equiv \theta \quad \forall \oplus \Sigma \oplus \emptyset \equiv \Delta \quad (3b)$$

Hence, these states will be called as "mixed" states. The 'impossible' state * of Eqn (1) can also be written as

$$\forall \otimes \Sigma \otimes \emptyset = * \quad (3c)$$

and it is never a state that is possible for the quantifier of a term.

The subsequent sections describe the machine QUANT-1, module-by-module, with brief theoretical explanations wherever necessary. The first few modules were built as individual units, but the later modules have been mounted on a metal chassis, as will be described later.

In what follows, a quantified term (QS) (e.g. "For all, true", or "Not for none, false") will be represented by its full 6-element form $(\zeta) (\gamma' \delta' \epsilon')$ $(\alpha \beta)$. As will be shown in section 7, every such statement has also a canonical form with only three elements $(\gamma \delta \epsilon)$. Until that section, we will discuss the implementation via circuits, of quantified statements only by the 6-element notation. It will consist of the "quantifier" $(\zeta) (\gamma' \delta' \epsilon')$ and the "term" $(\alpha \beta)$ to give a quantified term or statement.

2. QUANTIFIER INPUT MODULE (QIN)

This provides $(\gamma' \delta' \epsilon')$ and (ζ) as outputs to be used as inputs in other modules. The $(\gamma' \delta' \epsilon')$ output is available in a single 3-terminal socket, and any one of the 8 states mentioned in Table 1 can be selected by an 8-position rotary switch. The ζ output is available in a separate single-pin socket, and is set by an independent toggle switch. The panel layout is shown in Fig.1. The states employed in standard quantified logic are marked by circles.

3. TRANSFORMER MODULE (QTR)

This module performs a transformation operation on the general quantified term in the form of a six-element vector ;

$$[(\zeta) (\gamma' \delta' \varepsilon') (\alpha \beta)]$$

A set of four transformation operations have been defined in quantifier logic, viz., \mathcal{E}_E , \mathcal{E}_N , \mathcal{E}_M , \mathcal{E}_L . The effect of these on the eight quantifiers is given in Table 2. These operators are all, in fact, "identity" operations \mathcal{E} , ^{and} but only change the "description" of the QS, but not its logical content.

The transformations have been implemented by simple wire connections and inverters, as shown separately for each operator, in Fig.4. The implementation of all the 4 operators in a single module has been achieved by means of a 6-pole, 4-position rotary switch, as can be seen from the panel layouts shown in Fig.2 and Fig.3. One set of 3 sockets is provided on the module (Fig.2) for the outputs $(\zeta), (\gamma' \delta' \varepsilon'), (\alpha \beta)$ respectively for the purpose of comparison with another quantified vector, or any other use. In the later version of the transformer (Fig.3), two sets of outputs have been provided. A set of 6 lamps show the state of the components $(\zeta, \gamma', \delta', \varepsilon', \alpha, \beta)$ of the state transformed and outputted by this module. The ζ lamp glows red when ζ is 0, in order to denote the presence of a negation (\neg) of the quantification $(\gamma' \delta' \varepsilon')$, as explained in Section 1. A yellow lamp is also provided, which flashes when the $\underline{\underline{\alpha}}$ state is outputted for the SNS term $(\alpha \beta)$.

3.1. NOM circuit

At the time of construction of the module, it was felt that the effect of \mathcal{E}_N and \mathcal{E}_L on the $(\alpha \beta)$ components must be that of M when the $(\alpha \beta)$ input to the module is fed from Y or V modules of ESNY (instead of N, as shown in Table 2). For this purpose, the μ component was introduced as an additional input, which characterizes the ESNY module, i.e., assumes a value 1 for the modules Y and V,

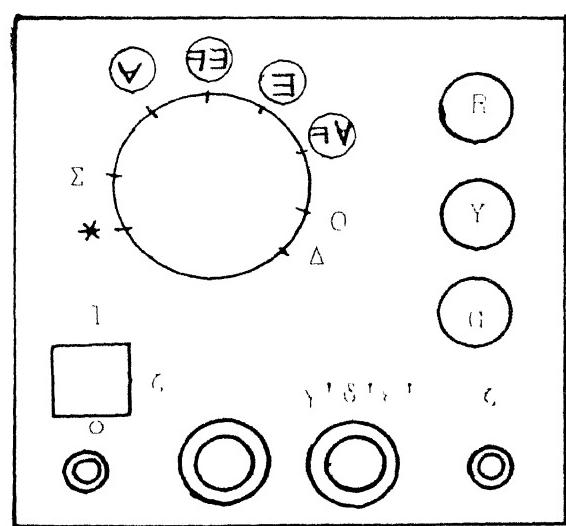


Fig.1. Quantifier Input (QIN)

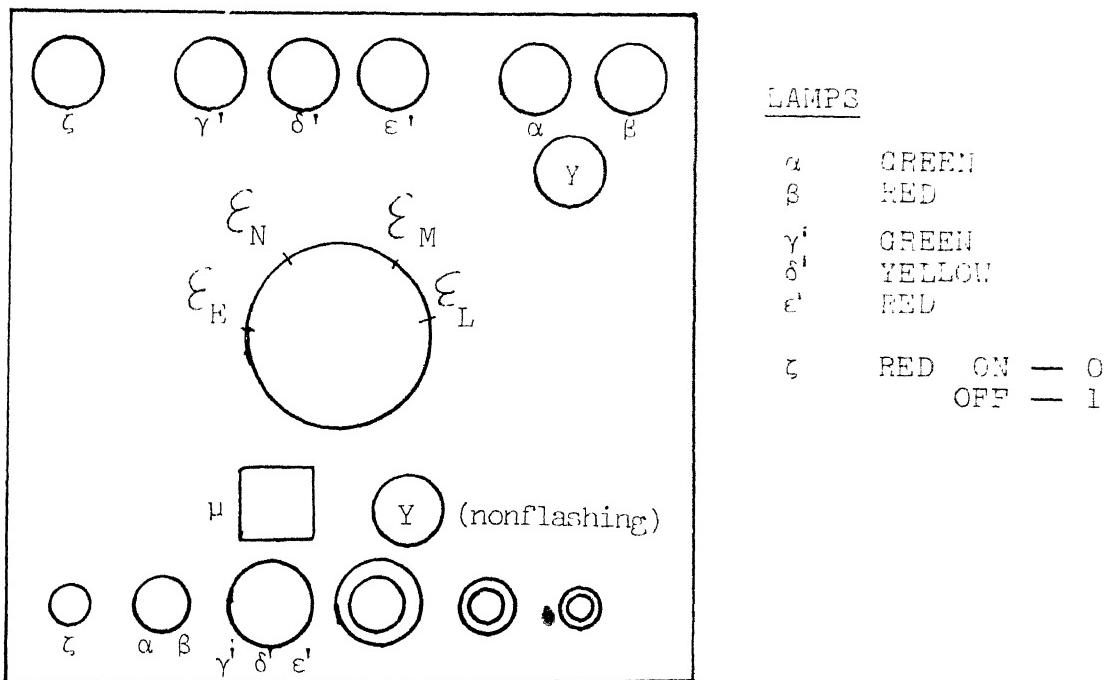


Fig. 2. Transformer (QTR) (First version)

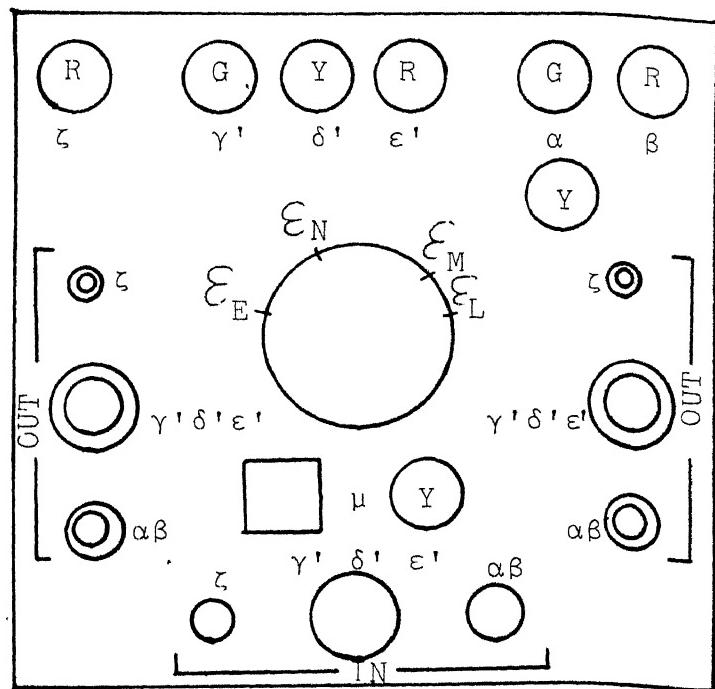


FIG. 3. TRANSFORMER (QTR) (Second Version)

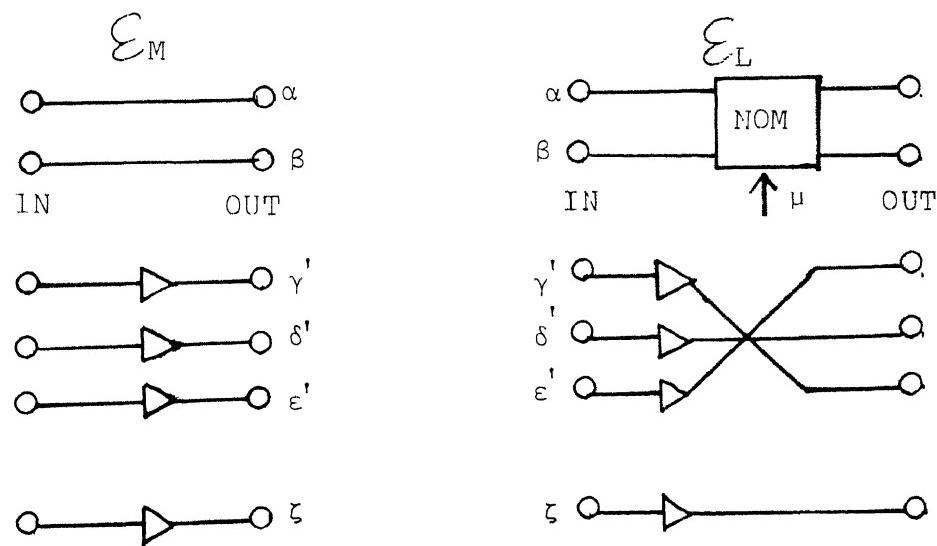
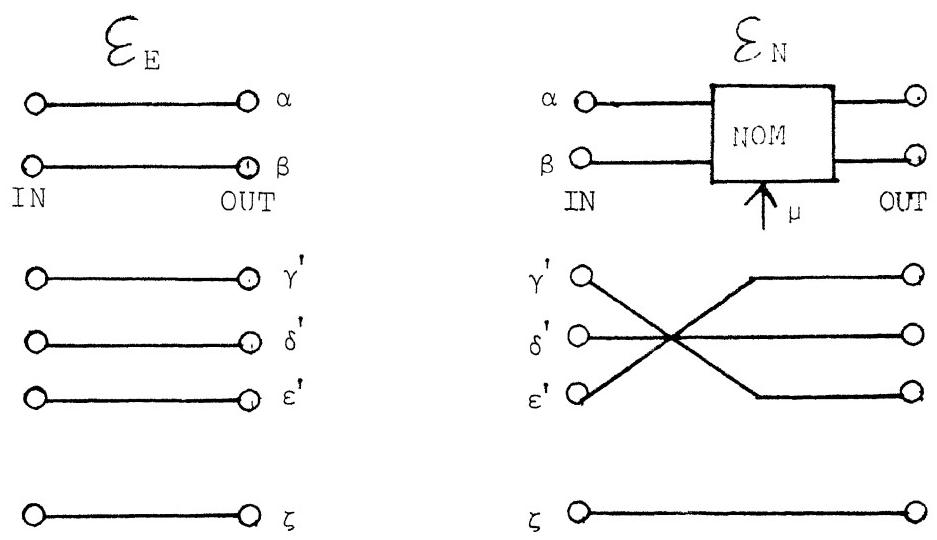


FIG. 4. QTR Wiring Diagram.

and is 0 for all other modules. The QTR modules shown in Figs. 2 and 3 have provision to produce the μ signal internally (by means of a switch) with a yellow lamp to indicate the state of μ 'on' for 1 and 'off' for 0. However, it was later found that the operator M is never used, and hence the μ singal is ignored, (i.e., it is always set to 0), since the effect of μ is to select the operator M only if $\mu = 1$, and to select the operator N, otherwise. The circuit for this selection, called the NOM circuit, is shown in Fig. 5.

4. QUANT COMPARISON MODULE (QG)

The module QG is designed to perform the operations of the operator QG which compares the 6-element state vector $\underline{Q_a}$ and $\underline{Q_b}$ of two quantified statements \underline{a} and \underline{b} . Representing these Boolean vectors by

$$\underline{a} = (a_\zeta) (a_\gamma, a_\delta, a_\varepsilon) (a_\alpha, a_\beta) \quad (4a)$$

$$\underline{b} = (b_\zeta) (b_\gamma, b_\delta, b_\varepsilon) (b_\alpha, b_\beta) \quad (4b)$$

a check is made in module for the equalities of the following single components:

$$\begin{aligned} a_\zeta &= b_\zeta \quad (a) ; \quad a_\gamma &= b_\gamma, \quad (b) ; \quad a_\delta &= b_\delta, \quad (c) \\ a_\varepsilon &= b_\varepsilon, \quad (d) ; \quad a_\alpha &= b_\alpha \quad (e) ; \quad a_\beta &= b_\beta \quad (f) \end{aligned} \quad (5)$$

QG will show a green light if all the equalities in (5) are satisfied, and a red light, even if one pair disagrees. This function has been implemented with a set of XOR gates, followed by a multiple NOR, as shown in Fig.7. The layout of the module QG is shown in Fig.6. The inputs are via three pin sockets, one each for (ζ), for ($\gamma, \delta, \varepsilon$) and for (α, β); the same can also be taken as outputs from the module. In addition the output of QG is available as an SNS vector $\underline{c} = (c_\alpha, c_\beta)$.

It is to be particularly noted that the output of QG is not a QS, but an SNS vector $\underline{c} = (c_\alpha, c_\beta)$, which can, of course, be quantified, when needed.

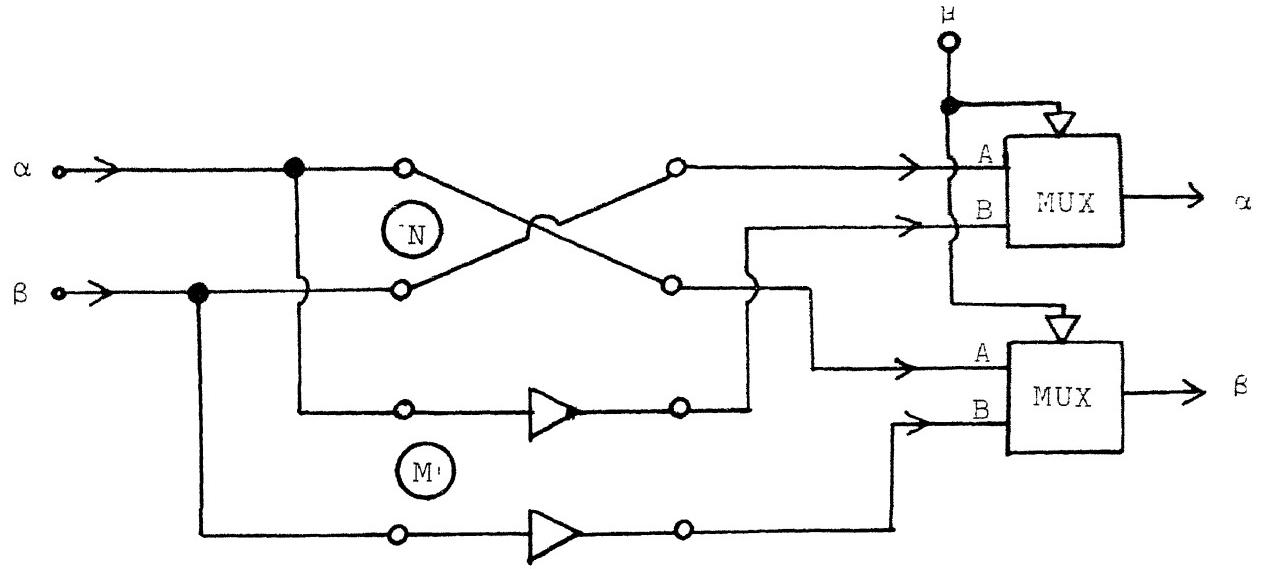


FIG.5. NOM CIRCUIT

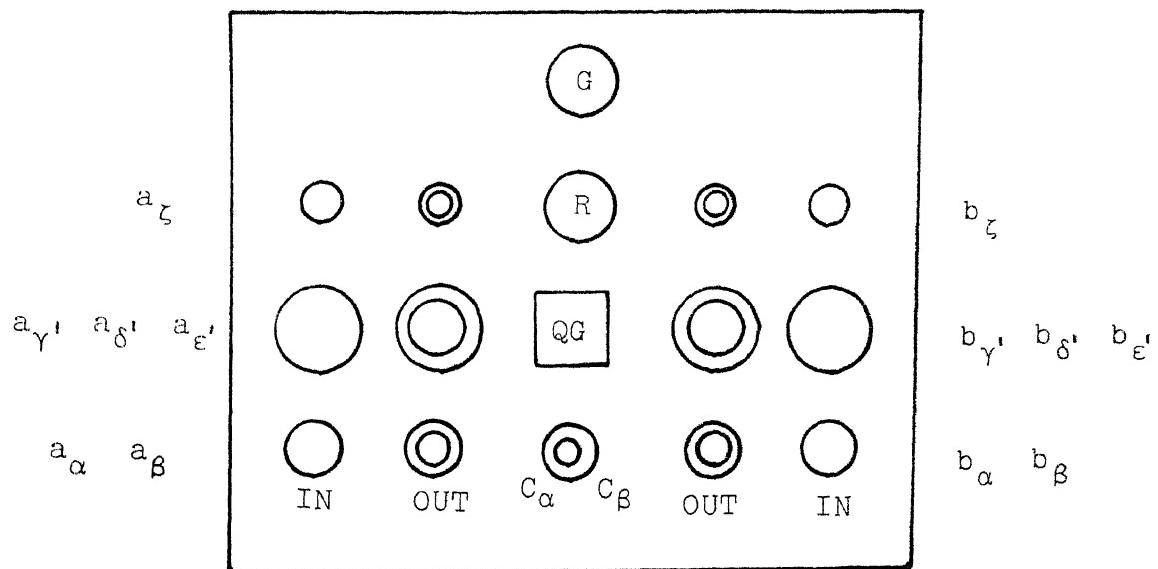


FIG.6. THE QUANT COMPARISON MODULE (QG)

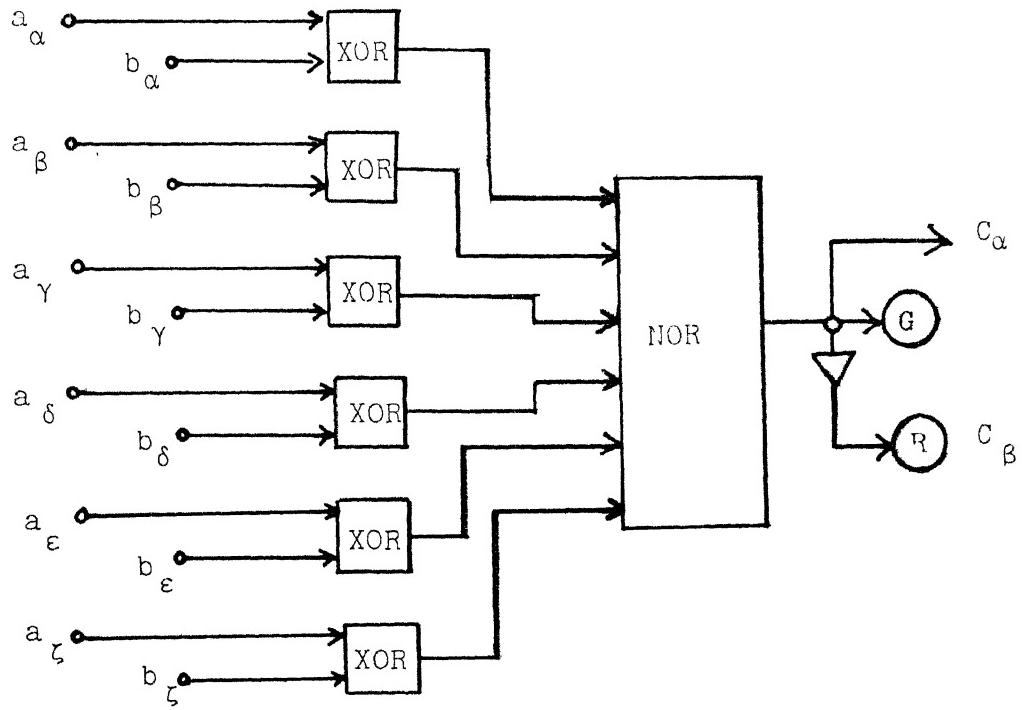


FIG. 7: CIRCUIT OF QG

5. QUANTIFIER-NORMALIZER MODULE (QN)

In standard first order quantified logic, only four out of the eight states possible for the quantifier are used — viz. \forall , \exists , $\neg\forall$, $\neg\exists$. We found that the computerization of these states with connectives is best done by selecting only 2 states out of these for the QS, viz. \forall and \exists . The four states are possible by having for the SNS terms \underline{T} or \underline{F} ($2 \times 2 = 4$).

The module for converting the four classical quantifier states into one of the above two is called the "normalizer" (QN), and this is done by applying one of the two equivalence operators \mathcal{E}_E or \mathcal{E}_N as necessary (which is indicated by the absence of a flashing red light when the setting is correct).

QN (layout diagram in Fig.8) can generate the four classical quantifier states \forall , \exists , $\neg\forall$, $\neg\exists$ and the SNS states (α β). (It also has provision to generate the μ signal.) A pair of toggle switches in the bottom left provide the SNS states for (α β), and a 3 pole-4 way rotary switch provides the quantifier states, while a single toggle switch can set μ to 1 or 0. The quantified state (Q_a) thus obtained (Fig.9a) can then be normalized by the \mathcal{E}_E or \mathcal{E}_N operator, selected by a 2-position sliding switch, whose operations is shown in Fig.9b (SW 1). The module can also accept the (α β) and the μ signals from an external source. A switch "EXT/SLF" (SW 2) of Fig.9(b) selects between the internal set, and the externally fed, signals. There are 6 display lamps on the module. The red lamp flashes to indicate presence of a \neg and the symbol \forall or \exists lights up indicating the nature of the quantifier. The SNS state (α β) is indicated by lamps as usual. (The green lamp flashes when the N/M switch is set in the wrong position. The N/M switch does not interfere with the operation of the module, but only indicates that the correct operator is used. Later the NOM circuit has been ignored, as mentioned earlier).

The procedure for normalization is as follows: After the quantifier is set on the rotary switch, only the sliding switch $\mathcal{E}_E/\mathcal{E}_N$ has to be set in that position in which the red lamp ceases to flash, when the output will be in the normalized form. The full circuit of this module is shown in Figs. 9(a) and 9(b). All the operations in Section 6 are made using the normalized output.

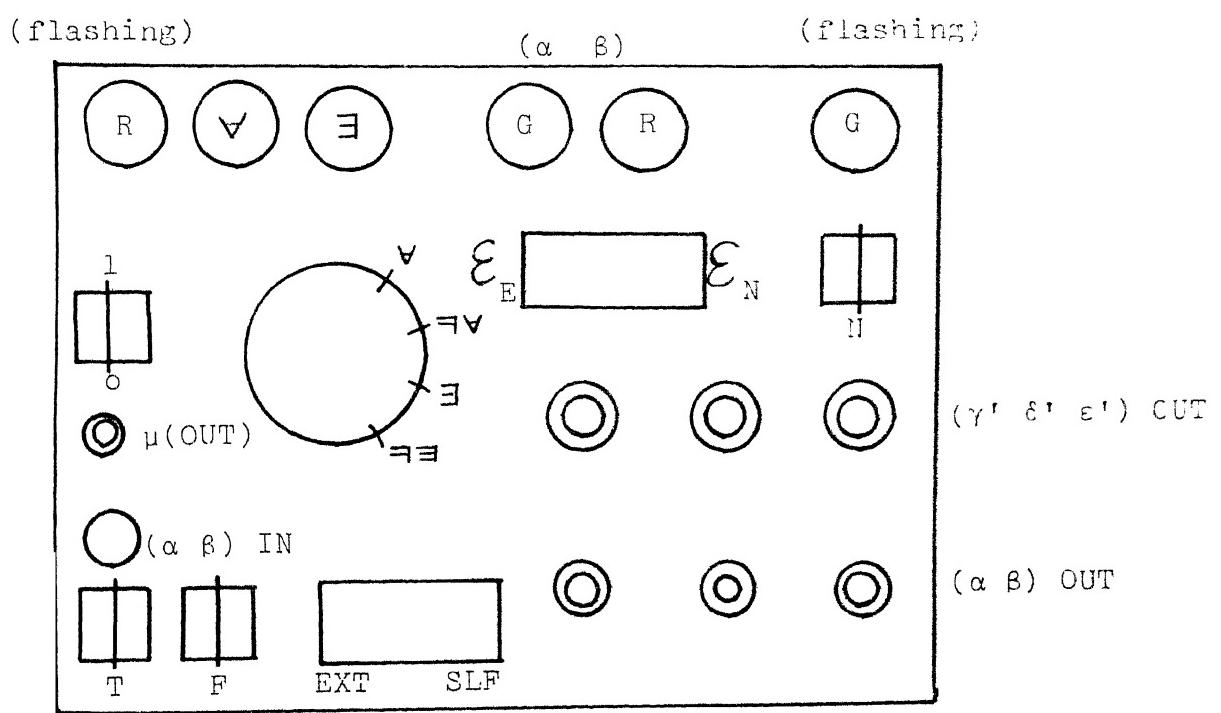
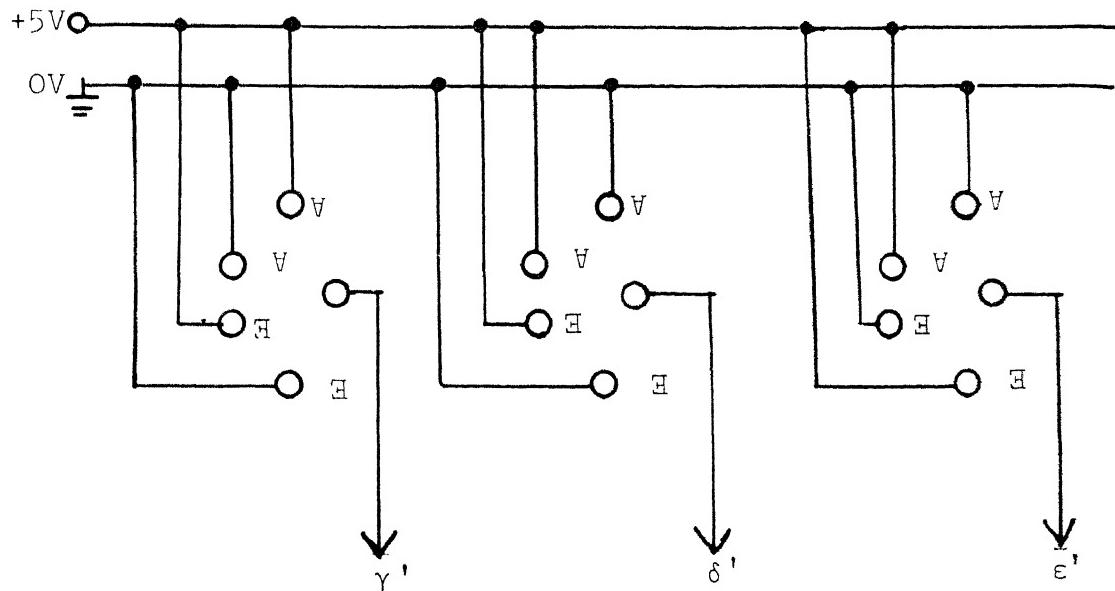


FIG.8. PANEL OF QN MODULE



to $\mathcal{E}_E/\mathcal{E}_N$ switch (SW1 of Fig.9b)

FIG.9(a) CIRCUIT OF QN

SWITCHES

SW1	: $\mathcal{E}_E/\mathcal{E}_N$ switch	sliding
SW2	: Ext/self (for μ, α, β)	
SW3	: T (α)	
SW4	: F (β)	
SW5	: N/M switch	toggle
SW6	: μ switch	

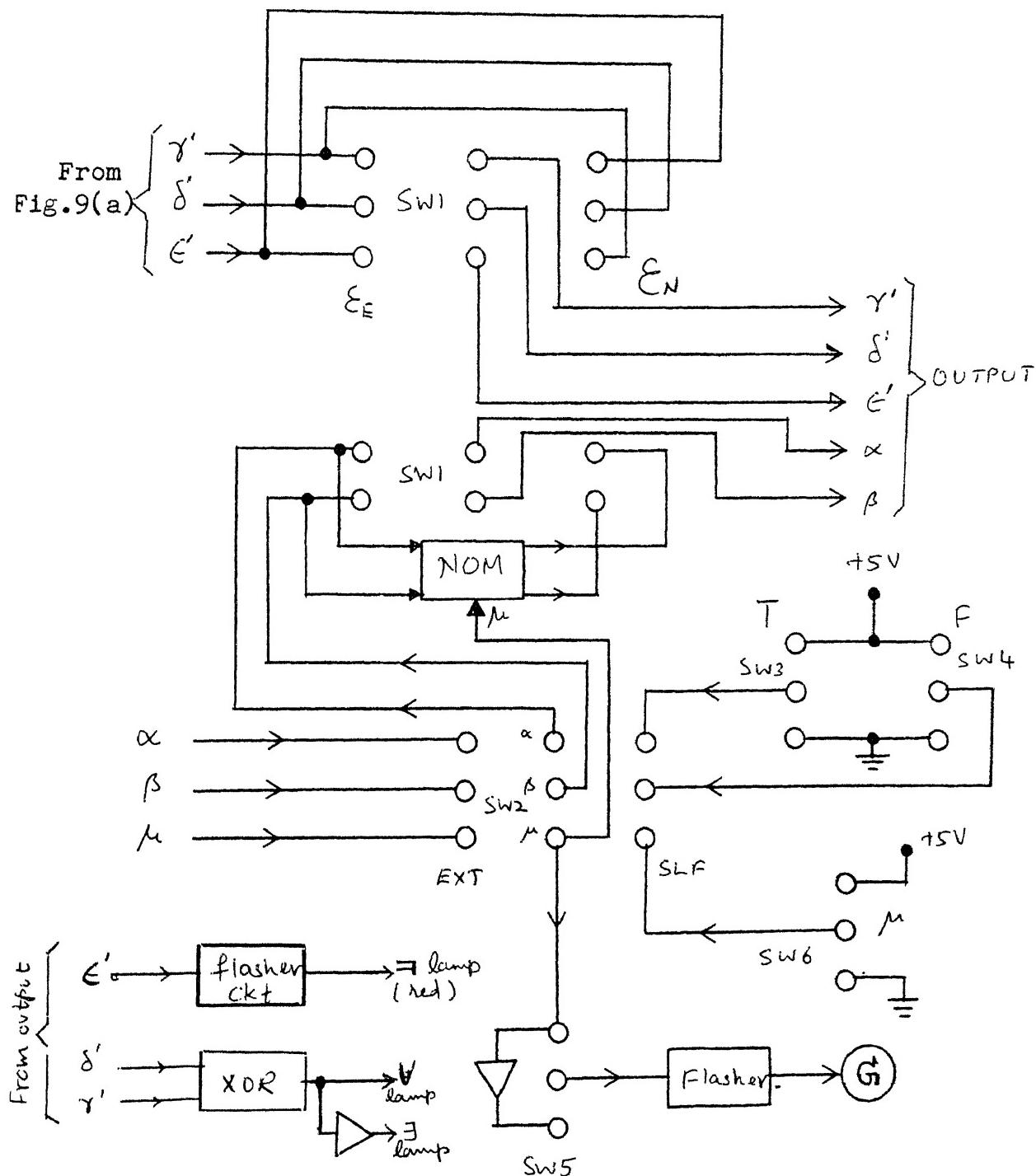


Fig. 9(b): QN CIRCUIT (contd)

6. QUANTIFIED BINARY CONNECTIVES (QBC)

The first inspiration for our study of connectives in quantifier logic came from the set of formulae given on page 117 of Howard DeLong's book "A Profile of Mathematical Logic", Addison-Wesley, 1971. In particular, the formulae given in set C on that page define the behaviour of "and" and "or" in quantifier logic, under the special conditions considered therein. These, translated into our terminology, provide the quantified binary relation:

$$\underline{a} \underset{\underline{m}}{\sim} \underline{b} = \underline{c} = (\underline{Q}'_c) (\underline{c}^i \underline{R}_0) \quad (5)$$

where

$$\underline{a} = (\underline{Q}'_a) (\underline{a}), \quad \underline{b} = (\underline{Q}'_b) (\underline{b}), \quad \underline{c} = (\underline{Q}'_c) (\underline{c}) \quad (5a)$$

$$\underline{c}^i = \underline{a} \underset{\underline{m}}{\sim} \underline{b} \quad (6)$$

and

$$\underline{R}_0 = \underline{R}_0 (\underline{Q}'_a, \underline{Q}'_b, \underline{Q}'_c, \underline{Z}) \quad (7)$$

Obviously, \underline{a} and \underline{b} are SNS terms and \underline{Z} is the SNS operator corresponding to the QUANT connective \underline{m} (i.e. of the same nature, namely "and" or "or"), and \underline{R}_0 can be one of three, namely \equiv , \Rightarrow , or \Leftarrow , which is applied to the "intermediate" SNS vector $\underline{c}^i = \underline{a} \underset{\underline{m}}{\sim} \underline{b}$. In our approach, the function of \underline{R}_0 is to modify \underline{c}^i to give \underline{c} , along with the quantifier state \underline{Q}'_c . However, the nature of \underline{R} depends on all the three quantifiers \underline{Q}'_a , \underline{Q}'_b , and \underline{Q}'_c and also on the nature of the connective \underline{Z} that is being considered, all of which will be provided, for working out \underline{c} in \underline{c} .

Using only the quantifiers \forall and \exists for \underline{Q}'_a , \underline{Q}'_b and \underline{Q}'_c , we worked out, from common sense, a table for \underline{R}_0 , for the QUANT connectives "and" (A) and "or" (O) (Tables 3(a), 3(b)), and started to implement the tables in electronics. The resulting modules were called "Set A" and "Set O". The module for the set A contains the connectives \underline{a} , \underline{I}^c , \underline{J}^c , \underline{O}^c , and the panel layout is shown in Fig.10. In this \underline{Q}'_a , \underline{a} , \underline{Q}'_b , \underline{b} are inputs and \underline{Q}'_c (also given) is set by the switch to be \forall or \exists , and it is displayed by lamps. The rotary switch chooses between A , \underline{I}^c , \underline{J}^c , \underline{O}^c , and the output, obtained using the internal logic circuitry, is \underline{c} (outputted as \underline{Q}_c , \underline{c}).

Table 3(a): Table of R_{\sim_O} for the QUANT connective \sim_A in $a \sim_A b$

Q'_a	Q'_b	Q'_c	R_{\sim_O}	Effective unary connective
A	A	A	\equiv	
A	A	E	\Rightarrow	
A	E	A	\Leftarrow	
A	E	E	\Rightarrow	
E	A	A	\Leftarrow	
E	A	E	\Rightarrow	
E	E	A	\Leftarrow	
E	E	E	\Leftarrow	

Table 3(b): Table of R_{\sim_O} for the QUANT connective \sim_O in $a \sim_O b$.

Q'_a	Q'_b	Q'_c	R_{\sim_O}	Effective unary connective
A	A	A	\Rightarrow	
A	E	A	\Rightarrow	
A	E	E	\Leftarrow	
A	E	E	\Rightarrow	
E	A	A	\Leftarrow	
E	A	E	\Rightarrow	
E	E	A	\Leftarrow	
E	E	E	\equiv	

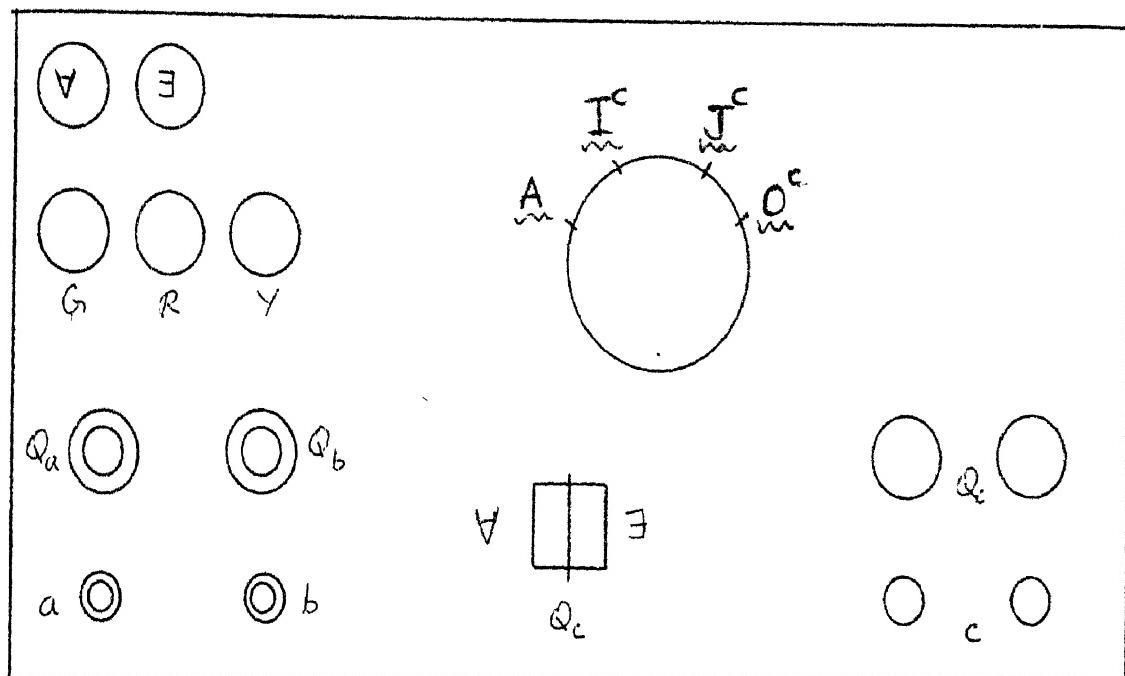


Fig.10: MODULE FOR THE SET A

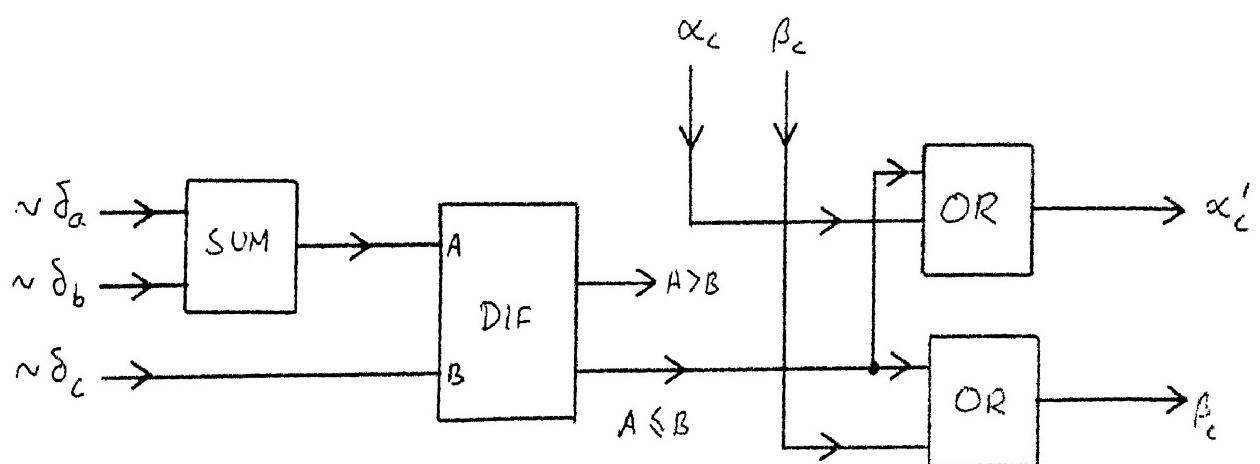


Fig.11: CIRCUIT OF A (R_0)

Table 4(a) shows the method of converting \underline{A} into \underline{I}^C , \underline{J}^C and \underline{O}^C , Fig.11 shows the \underline{A} circuit. The functioning of the circuit is as follows. The signals \underline{Q}'_a , \underline{Q}'_b and \underline{Q}'_c are used to produce the effective unary operation corresponding to $R_0 = \sim R_0(\underline{Q}'_a, \underline{Q}'_b, \underline{Q}'_c, \underline{Z})$ (as per Table 3(b)), which modifies $\underline{c} = (\underline{a} \sim \underline{b})$ accordingly. The functional details of the circuit are as follows. The quantifiers \forall and \exists are coded $V = 1$, $\exists = 0$; and $\sim \delta$ is used for representing this. The function used is $(\sim \delta_a \text{ AND } \sim \delta_b) - (\sim \delta_c)$. As shown in the circuit diagram of Fig.11, the effect of minus (-) in this function is obtained using the chip DIF which transmits a Boolean signal 1 in one of two lines according as the inputs A or B (binary numbers 0 to 4) is larger. The circuit used for $\sim R_0$ makes $\sim R_0 = \Rightarrow$ or \Leftarrow (both of which lead to E), and $\sim R_0 = \Leftarrow$ (leading to N), according as $A > B$ or $A < B$, so as to fit Table 3(a).

The module for the set \underline{Q} contains the connectives \underline{Q} , \underline{I} , \underline{J} , \underline{O}^C , and its panel is shown in Fig.12. The \underline{Q} circuit is shown in Fig.13, and it is similar to the \underline{A} circuit. The function used and the rule employed for $\sim R_0$ are different in this case, so as to fit Table 3(b), and is shown in Fig.13.

7. THE CANONICAL FORM OF A QUANTIFIED STATEMENT

When we tried to fit the Tables 3(a) and 3(b) with real examples for the derived connectives, we found them to lead to obviously inapplicable results, although Tables 3 and 4 are correct for the \underline{A} and \underline{Q} connectives themselves. After carefully studying the various possibilities, we came to the conclusion that it is the CANONICAL FORM \underline{Q}_a of the quantified vector $(\underline{Q}_a)(\underline{a})$ that has to be used as input into the QBC modules. The canonical form \underline{Q}_a of a quantified vector $(\underline{Q}'_a)(\underline{a})$ is defined as $(\underline{Q}_a)(\underline{T})$, where $(\underline{Q}_a)(\underline{T})$ is a logically equivalent form of $(\underline{Q}'_a)(\underline{a})$, obtained by applying the appropriate operator out of the four $(E_E, E_N, E_M \text{ or } E_L)$ on $(\underline{Q}'_a)(\underline{a})$. Table 5 gives the 3 canonical forms corresponding to the eight possibilities for \underline{Q}_a , and the four equivalent standard forms for each, obtained by applying the operations E_E, E_N, E_M and E_L to each of these. Hence, any QS, given in the standard notation $(\underline{Q}'_a)(\underline{a})$ has a unique canonical form \underline{Q}_a .

7.1. THE CANONIZER

A "canonizer" circuit incorporating the above ideas has been designed, which accepts the inputs $(\zeta) (\gamma' \delta' \epsilon')$ ($\alpha \beta$), of a QS, and automatically converts the description into the canonical form, which consists only of the components $(\gamma \delta \epsilon)$,

Table 4 : Conversion of \wedge and \vee into sets of four connectives

(a) Set "and"	(b) Set "or"	Operator acting on			
\wedge	\vee	\oplus_a'	\oplus_b'	\cong_a	\cong_b
\wedge	\vee	ϵ_E	ϵ_E	\sim_E	\sim_E
\wedge^C	\vee^C	ϵ_L	ϵ_E	\sim_N	\sim_E
\wedge^C	\vee	ϵ_E	ϵ_L	\sim_E	\sim_N
\wedge^C	\vee^C	ϵ_L	ϵ_L	\sim_N	\sim_N

Table 5 : Possible Standard Forms of Quantified Statements
corresponding to the Eight Canonical Forms

Canonical Form \underline{Q}_a $(\gamma \delta \epsilon)$	Equivalent Standard Forms $(\underline{Q}_a)(a) = (\zeta)(\gamma' \delta' \epsilon')(a \beta)$			
	ϵ_E	ϵ_N	ϵ_M	ϵ_L
$\forall (1 \ 0 \ 0)$	$\forall (a_T)$	$\emptyset (a_F)$	$\exists \forall (a_T)$	$\exists \exists (a_F)$
$\emptyset (0 \ 0 \ 1)$	$\emptyset (a_T)$	$\forall (a_F)$	$\exists \exists (a_T)$	$\exists \forall (a_F)$
$\exists (1 \ 1 \ 0)$	$\exists (a_T)$	$\forall (a_F)$	$\exists \emptyset (a_T)$	$\exists \forall (a_F)$
$\wedge (0 \ 1 \ 1)$	$\wedge (a_T)$	$\exists (a_F)$	$\exists \forall (a_T)$	$\exists \emptyset (a_F)$
$\Sigma (0 \ 1 \ 0)$	$\Sigma (a_T)$	$\Sigma (a_F)$	$\exists \theta (a_T)$	$\exists \theta (a_F)$
$\theta (1 \ 0 \ 1)$	$\theta (a_T)$	$\theta (a_F)$	$\exists \Sigma (a_T)$	$\exists \Sigma (a_F)$
$\Delta (1 \ 1 \ 1)$	$\Delta (a_T)$	$\Delta (a_F)$	$\exists \exists (a_T)$	$\exists \exists (a_F)$
$\times (0 \ 0 \ 0)$	$\times (a_T)$	$\times (a_F)$	$\exists \Delta (a_T)$	$\exists \Delta (a_F)$

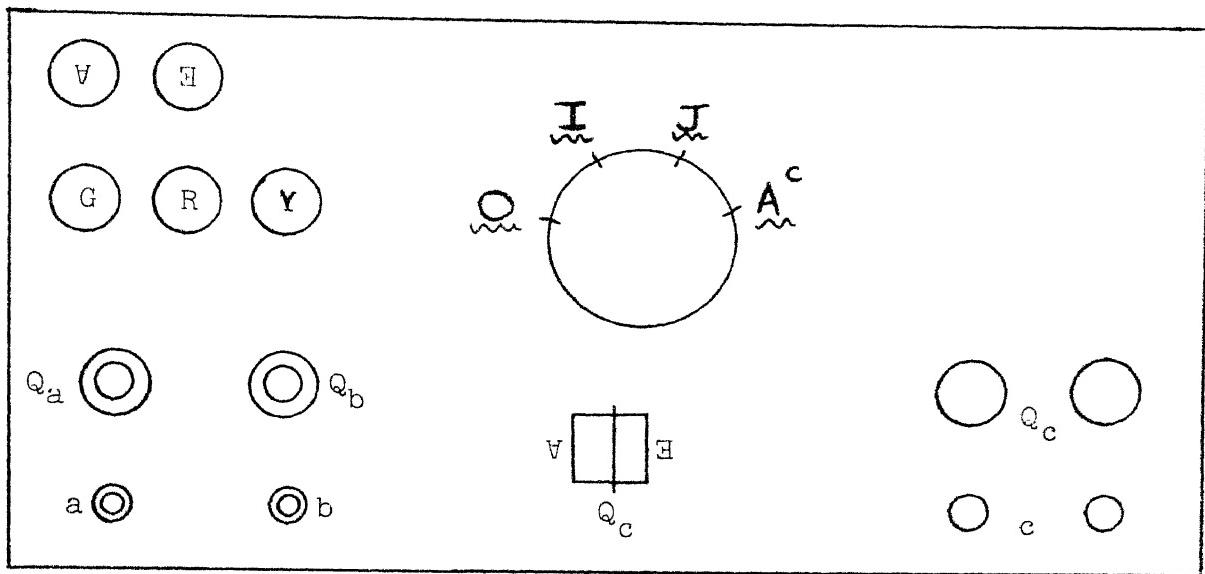


FIG.12. MODULE FOR THE SET O

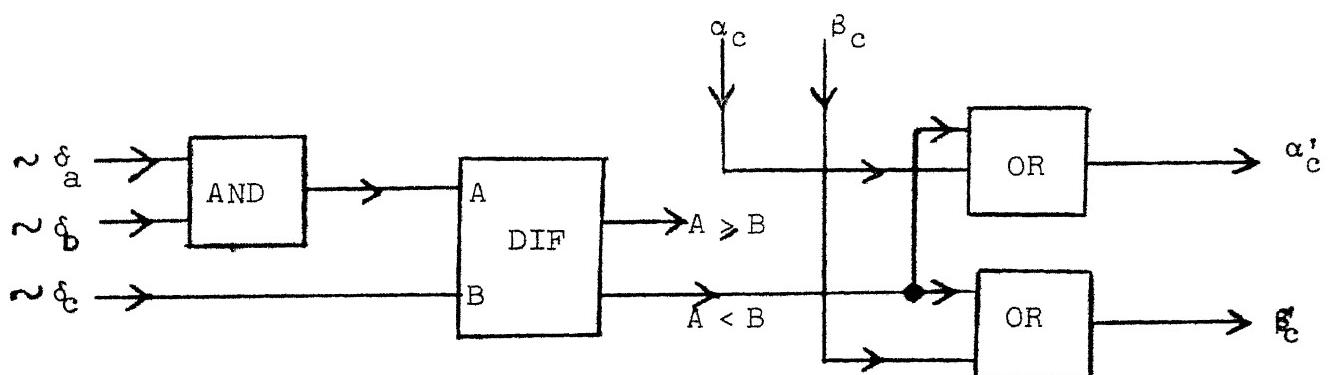


FIG.13. CIRCUIT OF O (R_O)

with ζ assumed to be 1, and $(\alpha \beta)$ always being taken to be $(1 \ 0) = \underline{T}$. Consequently, it requires only three Boolean elements $\gamma, \delta, \varepsilon$ for its description. The full circuit is shown in Fig.14(b), and the schematic is shown in Fig.14(a).

Considering Fig. 14(a), its working is readily explained by the following:

INPUT $(\zeta)(Q')(\alpha \beta)$, $Q' = (\gamma' \delta' \varepsilon')$

MUX 1 makes $\underline{Q}'_1 = Q'$, if $\zeta = 0$
and $= \underline{Q}'M$, if $\zeta = 1$

MUX 2 makes $\underline{Q}'_2 = *$ if $\alpha = 0$
and $= Q'$ if $\alpha = 1$

MUX 3 makes $\underline{Q}'_3 = *$ if $\beta = 0$
 $= \underline{Q}'_1 M$ if $\beta = 1$

PLUS makes $Q_{mn} = \underline{Q}'_2 \oplus \underline{Q}'_3$

In Fig.14(a), the effects of MUX 1 are produced by three MUX elements, while those of MUX 2 and MUX 3 are implemented by three "AND" gates for each. Finally the Boolean sum \oplus to give γ, δ and ε are obtained using three "or" gates.

A computer program to convert from the standard form of any QS input to its canonical form has also been written.

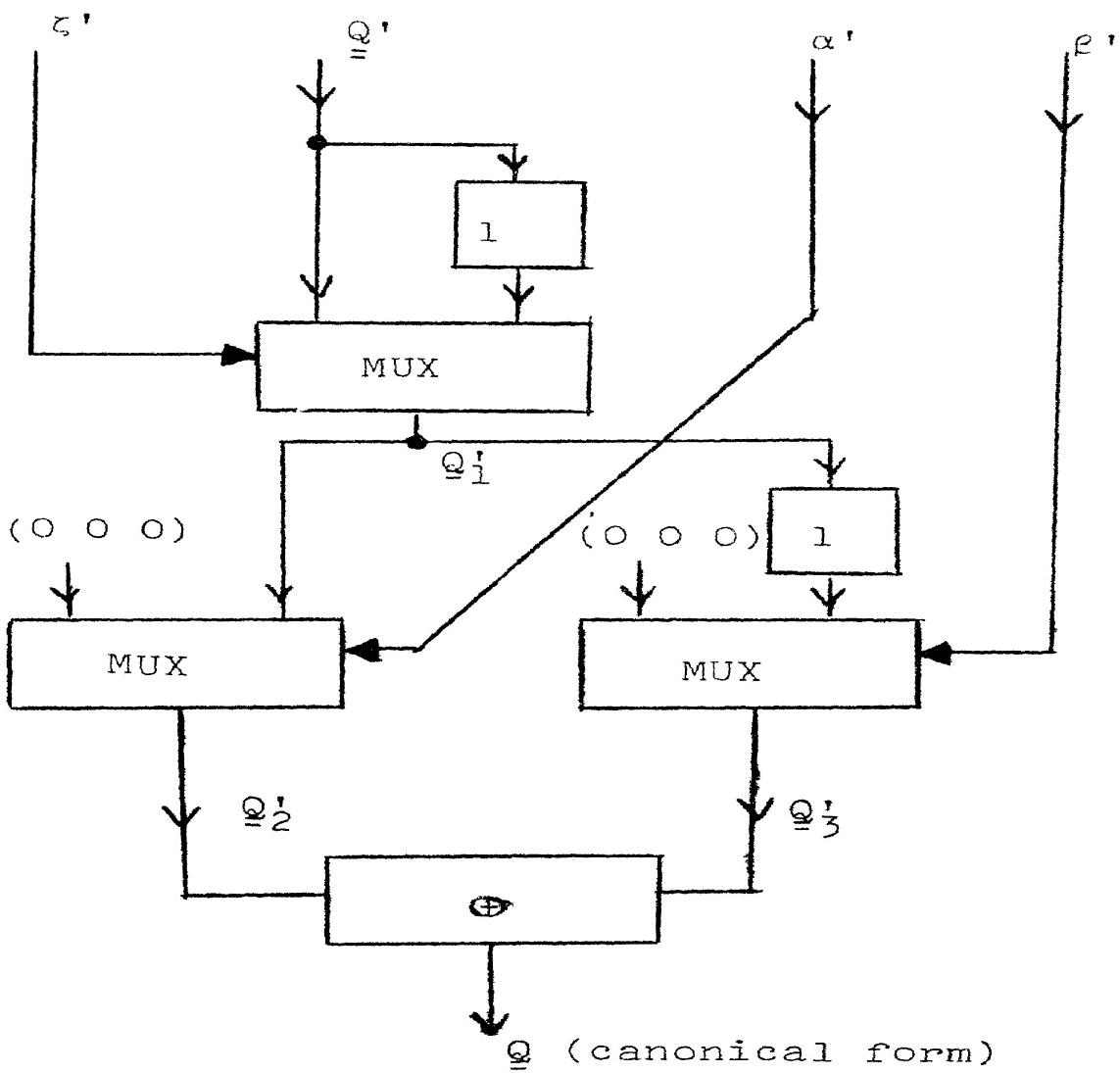


Fig. 14(a). SCHEMATIC OF THE CANONIZER

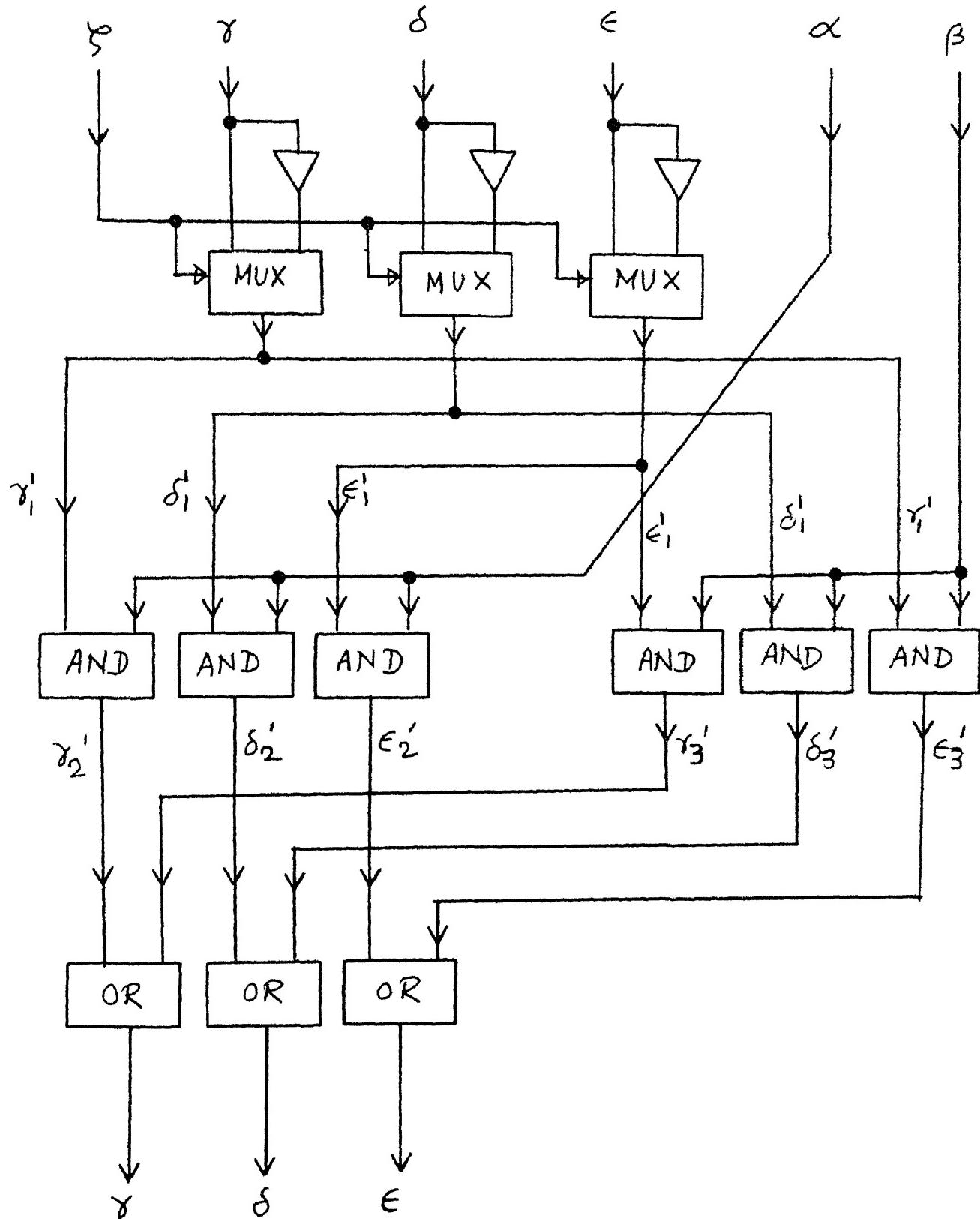


Fig. 14(b). CANONIZER (Full circuit)